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Title: The Ghosts of SimCCS: Past, Present, and Future

Author(s): Middleton, Richard Stephen

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Los Alamos

NATIONAL LABORATORY

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The Ghosts of *SimCCS*

Past, Present, and Future

Richard S. Middleton

10/1/2018

Key Partners

Developers

- Richard Middleton, Brendan Hoover (Los Alamos).
- Sean Yaw (Montana State University).
- Kevin Ellett (Indiana University; IU).

Users/publishers

- Jeff Bielicki (The Ohio State University).
- Andres Clarens (University of Virginia).
- Adam Brandt (Stanford University).
- Mike Kuby, Jorge Sefair (Arizona State University).
- Sam Taylor (University of West Virginia).

Current Los Alamos projects

- US-China “Clean Coal” CERC.
- DOE Regional Partnerships.
- DOE CarbonSAFEs (~10 for Los Alamos and IU)
- *SimCCS*: Development and Applications

Institutions

- Southern Company
- Great Plains Institute
- Chinese Academy of Sciences

BACKGROUND

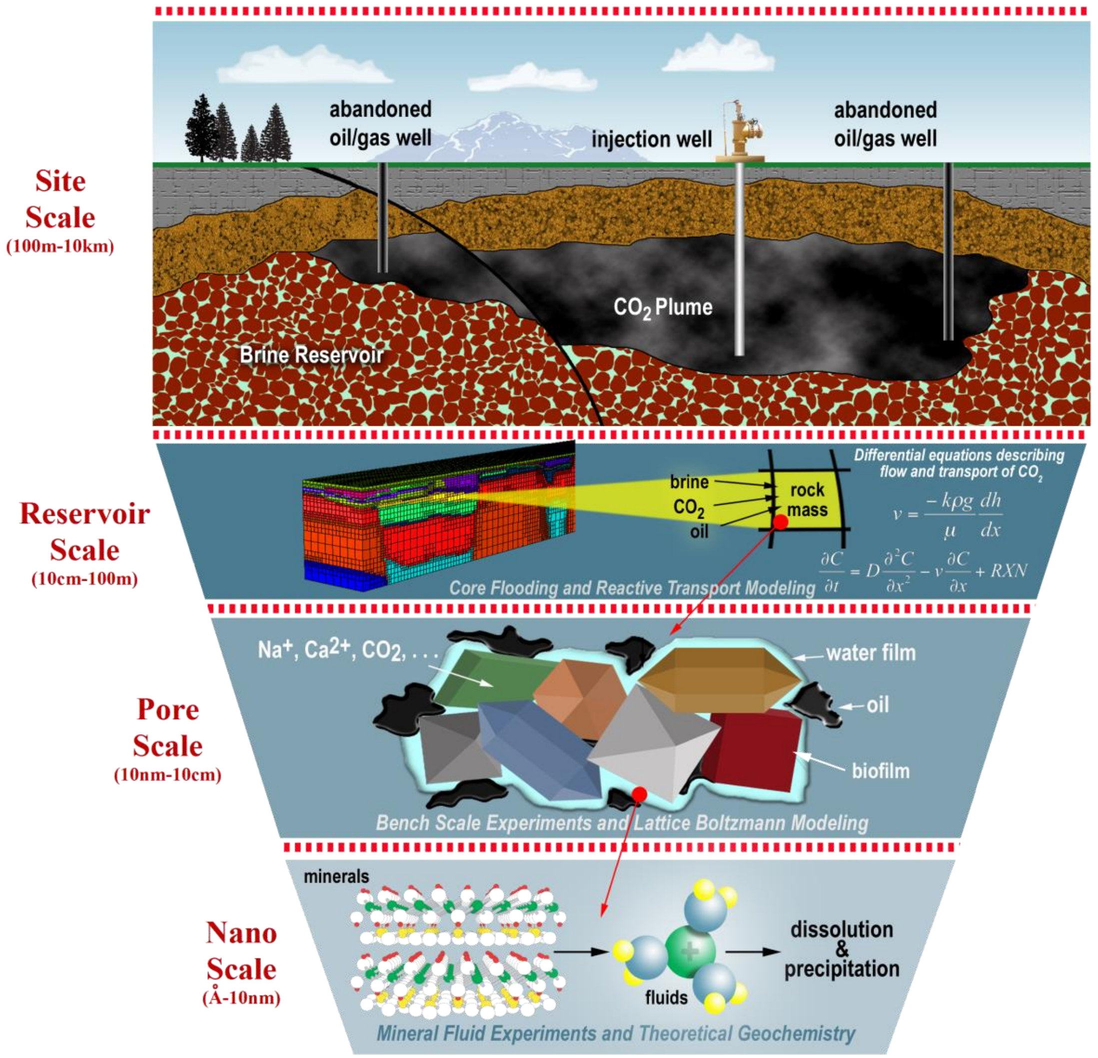
SimCCS Origins

Earth and Environmental Sciences

- Applied long history of flow & transport on porous media to carbon sequestration.
- Scales ranging from pore to site scale.
- Full-physics and reduce order modeling.
- Only a limited focus on capture.

CO_2 capture and transport (CCS)

- Classic source-network-sink optimization problem.
- Postdoctoral research work (2006)



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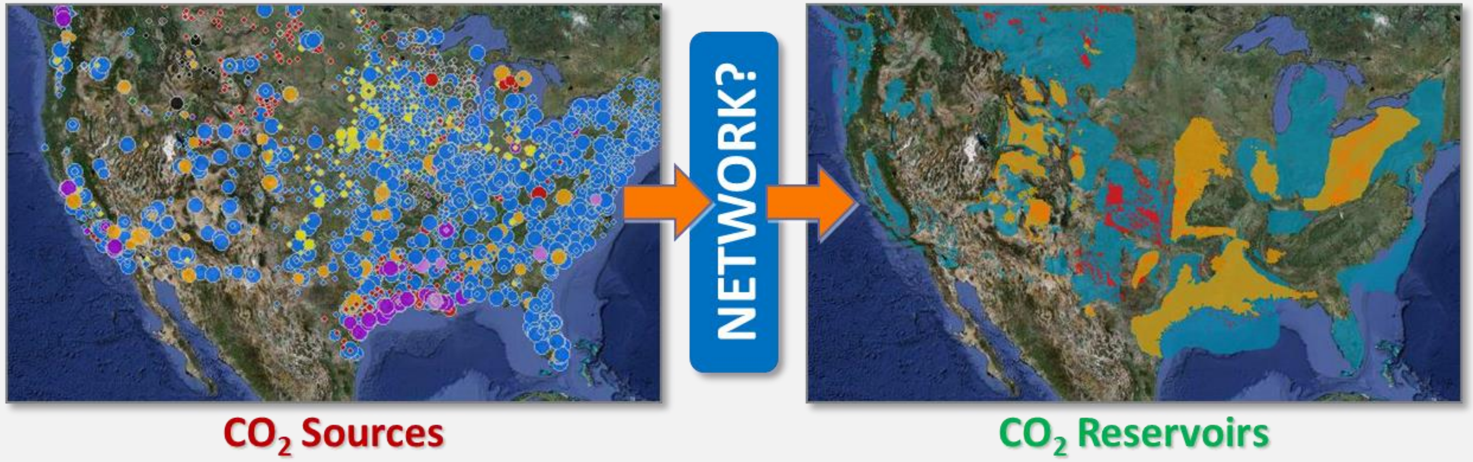
Simultaneously and optimally decide:

1. which CO_2 sources should be *built* or capture *retrofitted*
2. how much CO_2 to *capture* and *emit* at selected sources
3. which geologic reservoirs to *characterize* and *open*
4. how much CO_2 to *inject* and *store* in each reservoir
5. where to construct pipeline *network* with *trunklines*
6. what *discrete* capacity pipeline to build
7. how to *distribute* CO_2 (supplies/demands/transport)



Middleton and Bielicki (2009) A scalable infrastructure model for carbon capture and storage: *SimCCS*, *Energy Policy*

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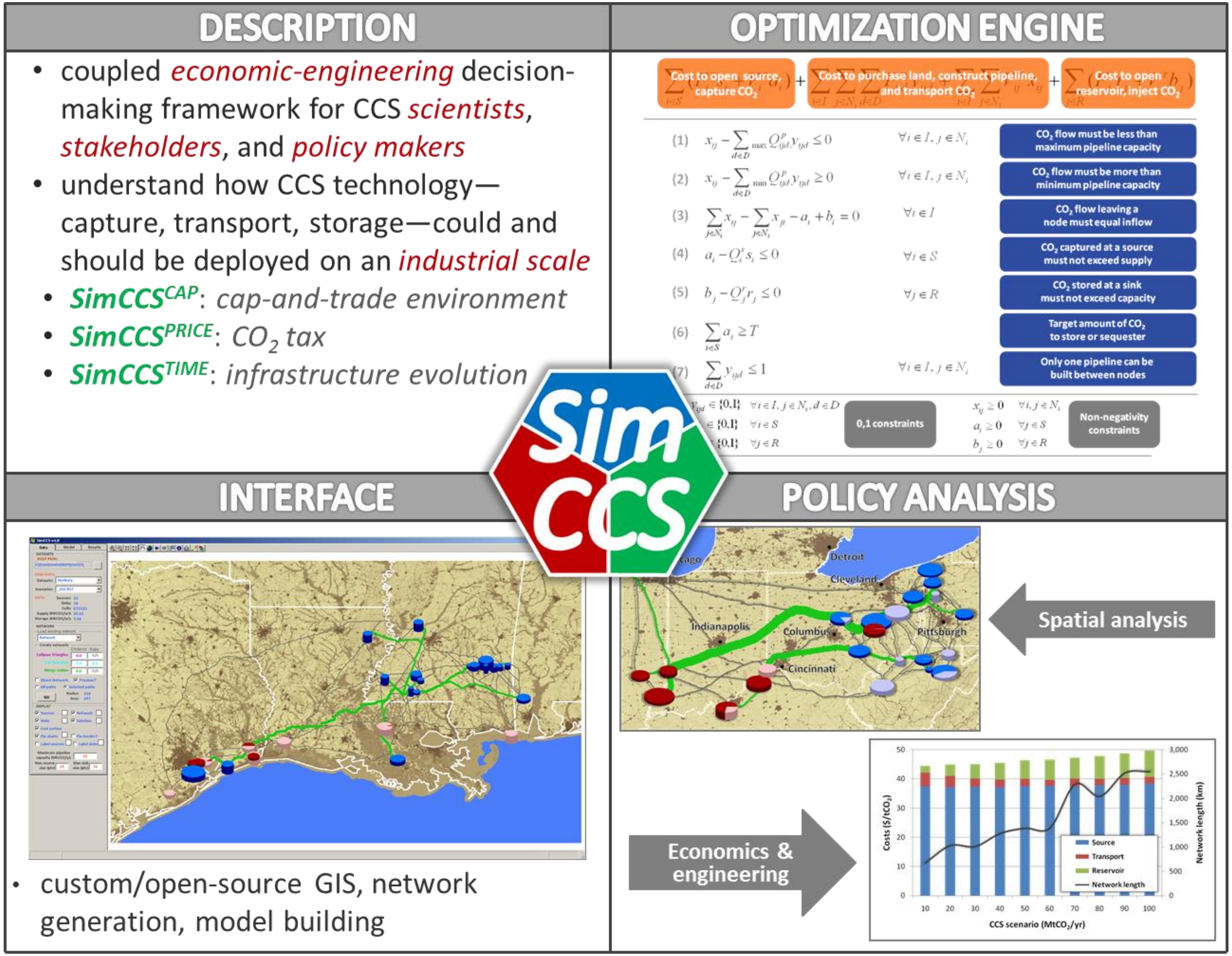
Background
SimCCS

SimCCS Framework
- Optimization engine.
- Integrated capture, transport, and storage models that define economical and engineering parameters.

Capture
- Literature values.
- IECM model (costs, CO_2).

Transport
- Cost surface.
- Candidate network.

Storage
- Reduced order model (CO_2PENS).
- Custom cost model.



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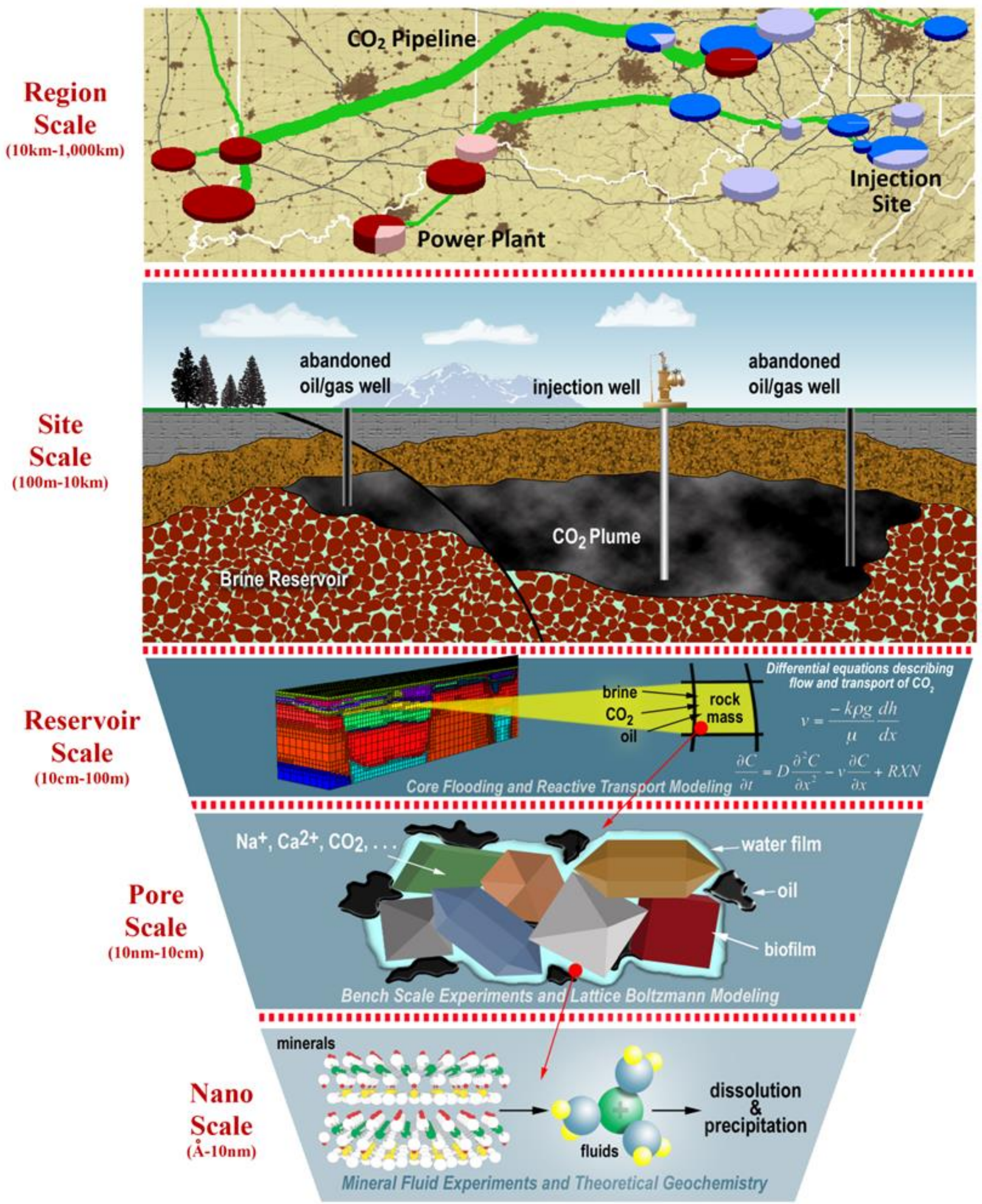

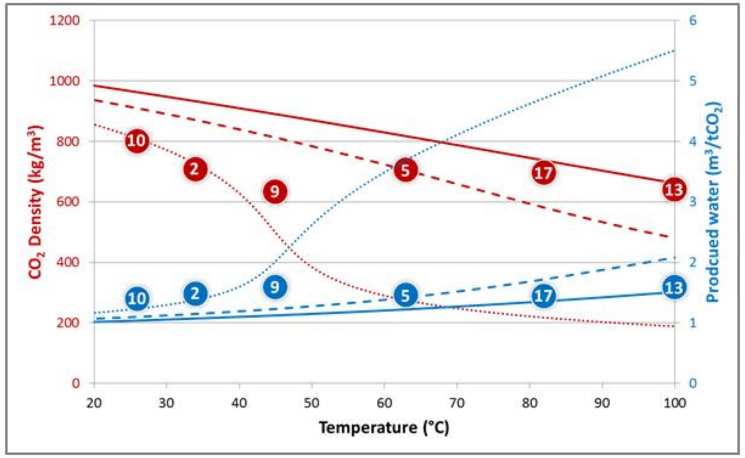

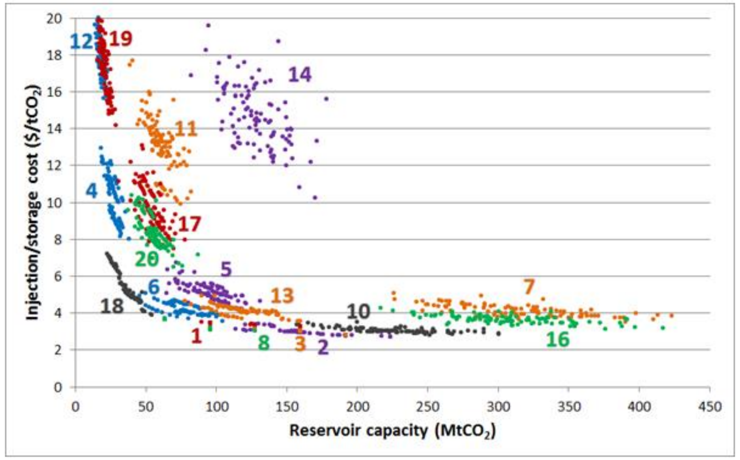

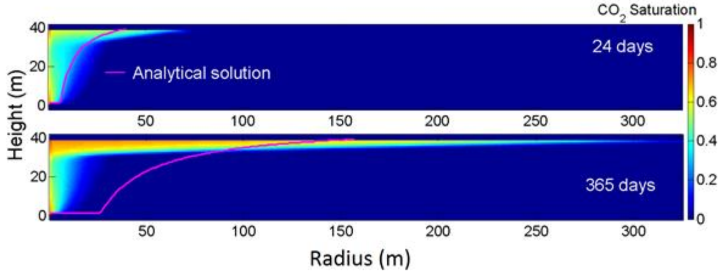

RAL

O2 cost-
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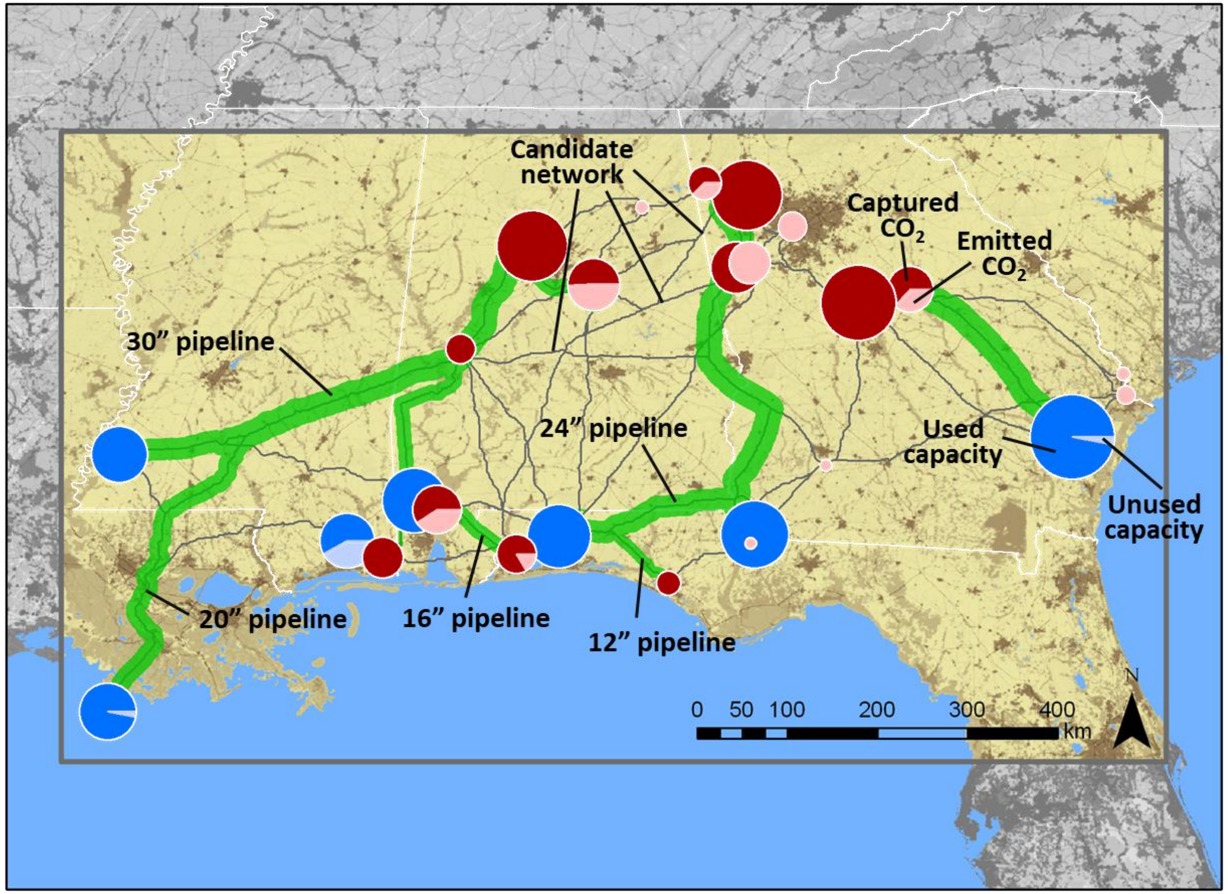
(1) *SimCCS*^{CAP}

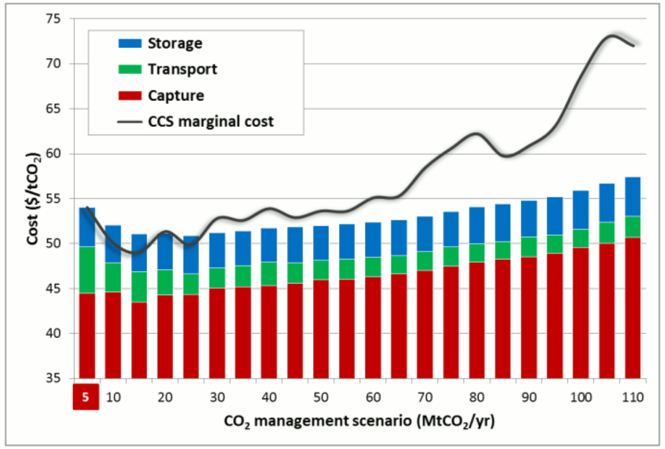
Original model

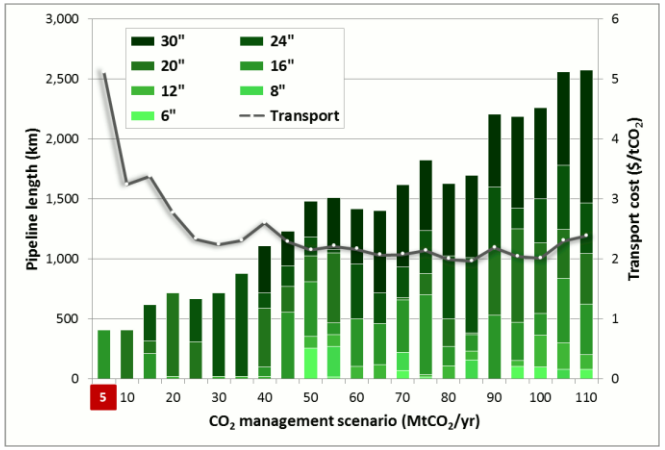
- Cap-and-trade version of *SimCCS* → set CO_2 cap (or target) & minimize costs.
- Inverse: set economic cap and maximize CO_2.

Southern Company

- Ten year business plan and CO_2 emissions strategy.
- 20 coal-fired plants, 156 $MtCO_2/yr$ emissions.
- 65 individual boilers→ boiler level accuracy.
- **CAPTURE COSTS:** \$46-102/tCO_2 (plant) & \$41-166/tCO_2 (boiler).
- **STORAGE:** 3.4 $GtCO_2$ in 7 sinks, 113 $MtCO_2/yr$ over 30 years.
- **STORAGE COSTS:** \$3.78-8.60/tCO_2.







Middleton *et al.* (2012) The cross-scale science of CO_2 capture and storage: from pore scale to regional scale, *Energy & Environmental Science*

MODELS/APPLICATIONS

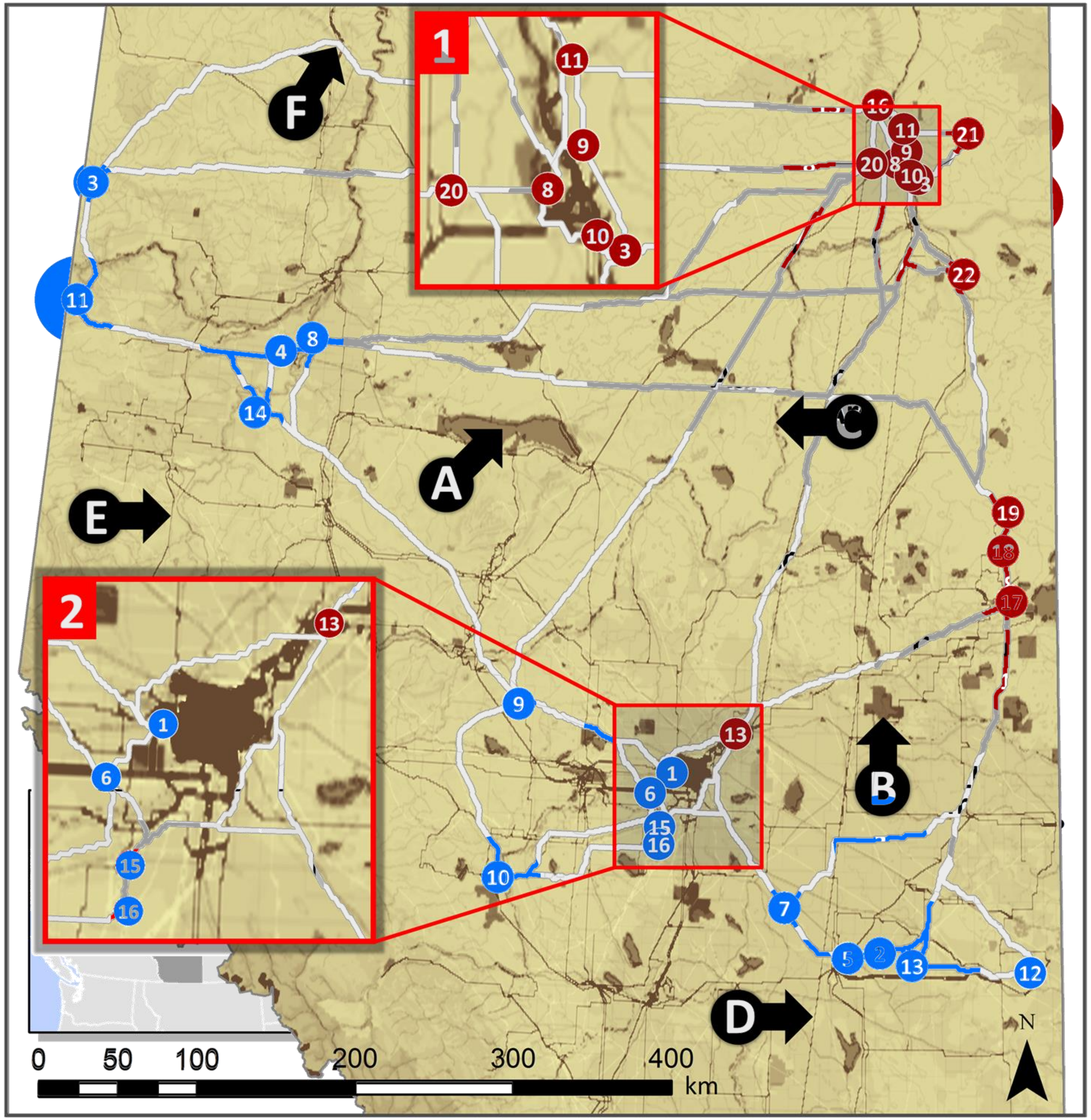
(2) *SimCCS*^{TAX}

Alberta oil sands

- *In situ* extraction, surface mining, & upgrading.
- 22 sources emitting 40 $MtCO_2$/yr, 36 $MtCO_2$/yr at 90% capture rate.
- 16 reservoirs (acid gas injection) with 2.5 $GtCO_2$ storage capacity.

Cost surface

- Detailed explanation of geography contributing to cost surface.
- First non-US cost surface (others now include France and China).



Middleton and Brandt (2013) Using infrastructure optimization to reduce greenhouse gas emissions from oil sands extraction and processing, *Environmental Science and Technology*

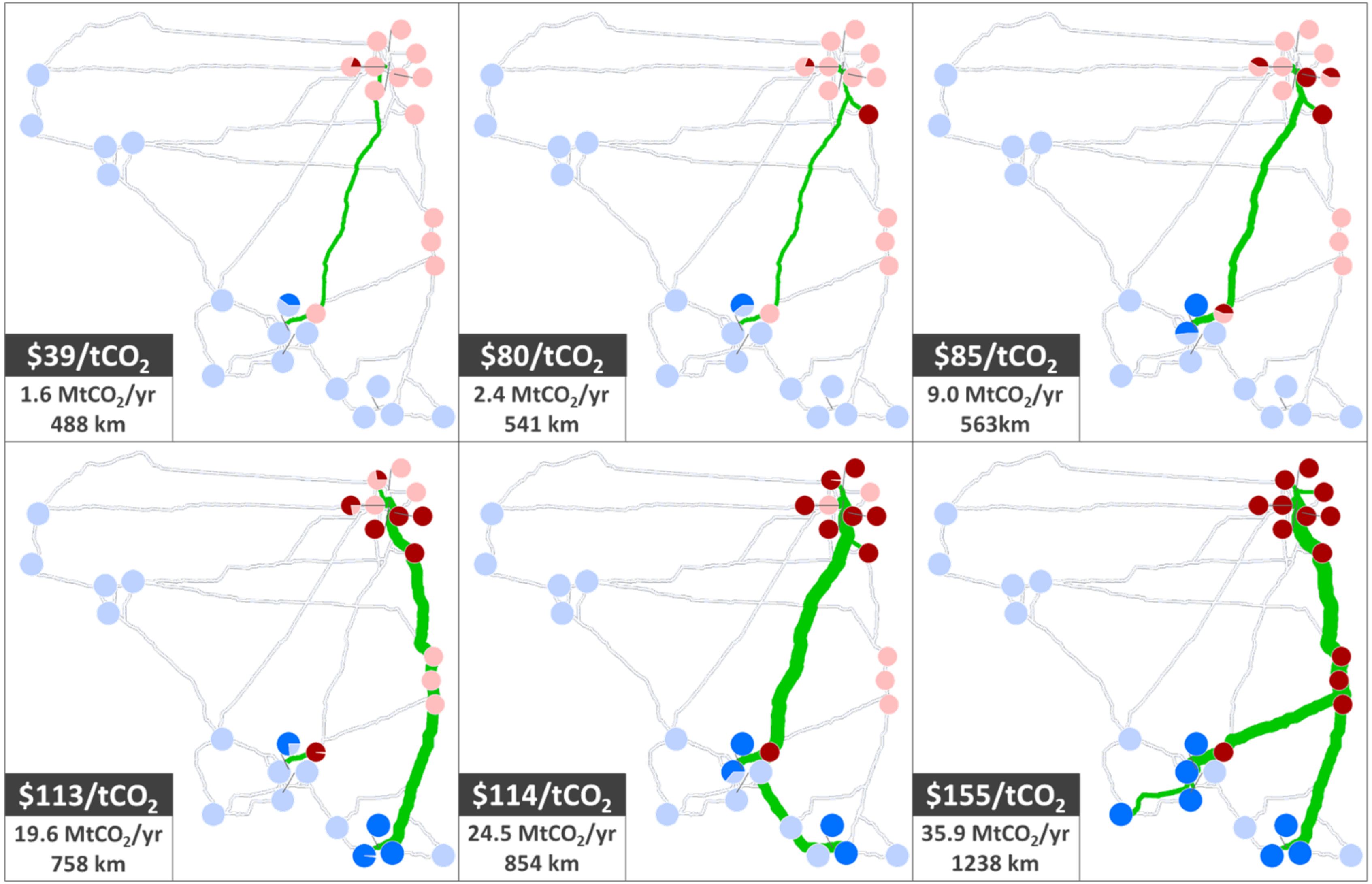
(2) *SimCCS*^{TAX}

Impact of a CO_2 tax

- *SimCCS* reformulated to account for CO_2 emission price.
- Minimizes costs, sources only capture if avoiding CO_2 tax is profitable.
- Direct application to "45Q".

Increasing CO_2 tax

- Infrastructure response to economic incentives.
- Drives increasing CO_2 capture rates and emissions reduction.



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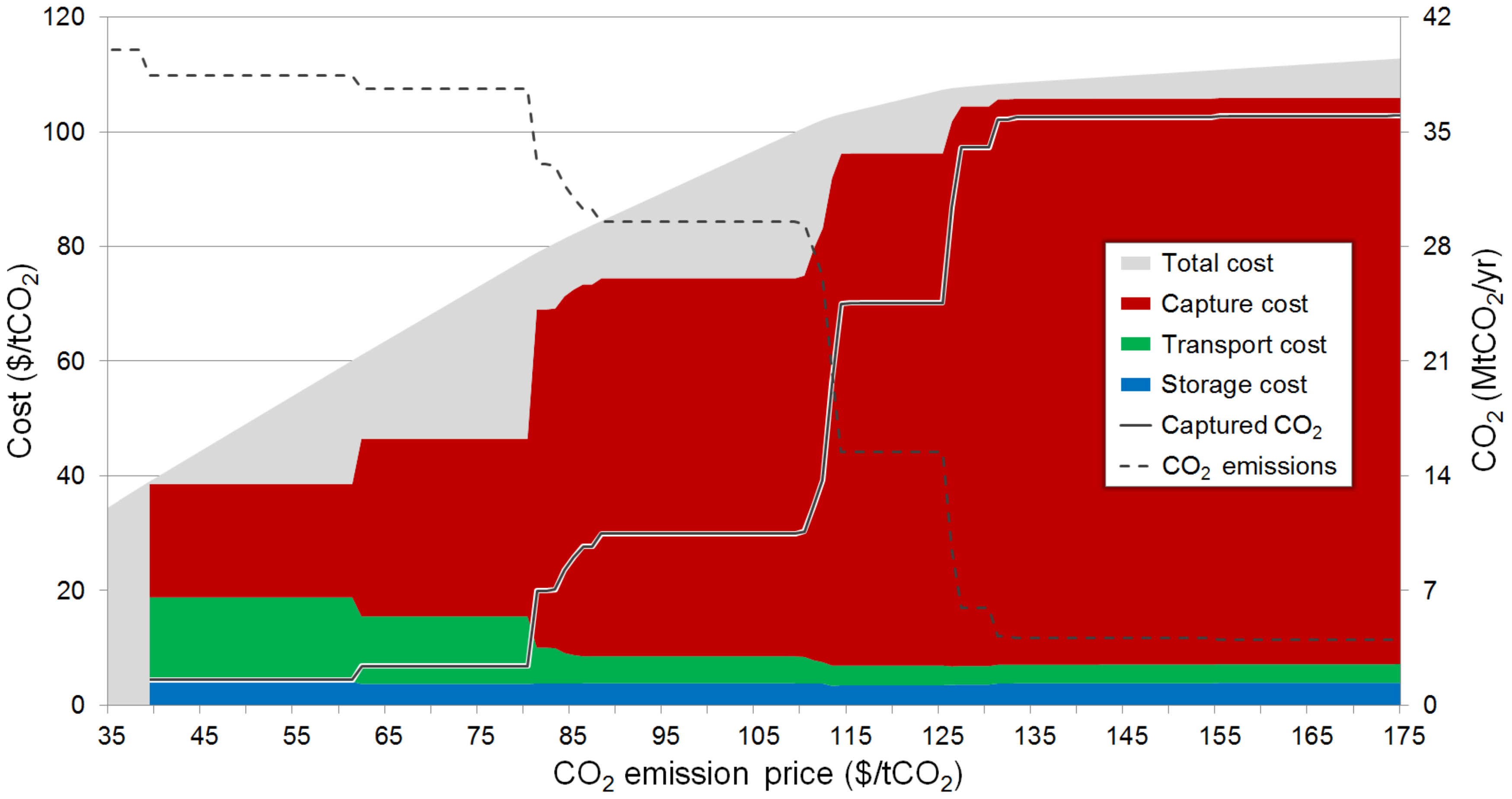

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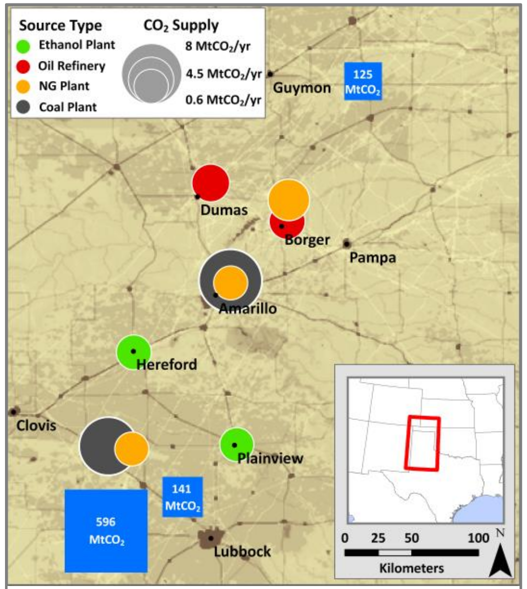
(3) SimCCS^{TIME}

Temporal dynamics

- *SimCCS^{TIME}*
- Synthetic dataset based on Natcarb

Results

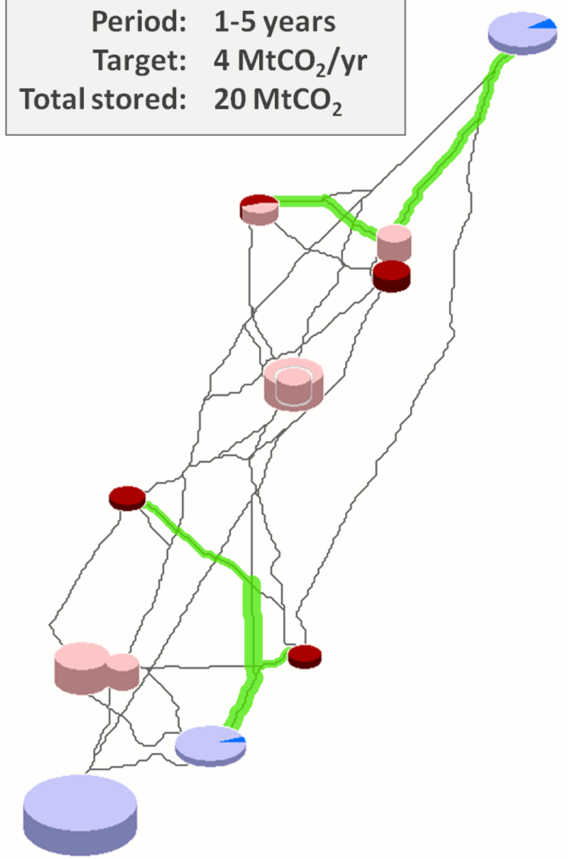
- Reduced costs by over-building infrastructure (i.e., underusing infra-structure for 5+ years).
- Significant economic gains from cooperation, particularly for small emitters.

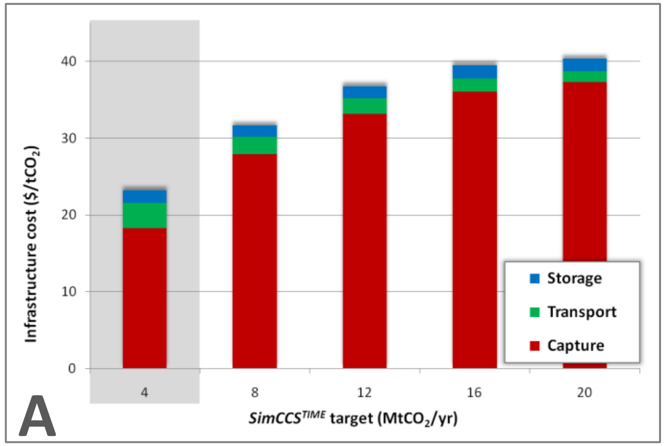


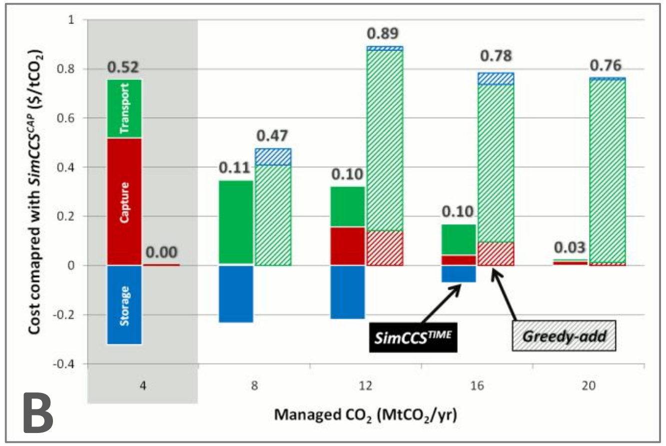
Texas panhandle

- 9 CO_2 sources (2 biorefineries, 2 oil refineries, 2 coal and 3 natural gas stations) producing 21 $MtCO_2$/yr
- 3 sequestration reservoirs (depleted oil fields) with 862 $MtCO_2$ capacity

Period: 1-5 years
Target: 4 $MtCO_2$/yr
Total stored: 20 $MtCO_2$







SimCCS^{TIME}

- *spatial optimization framework* for CO_2 capture and storage (CCS) infrastructure (capturing, transporting, injecting/storing CO_2) through *multiple time periods*
- deploys CCS *networks* to meet a CO_2 *cap* (i.e., cap-and-trade) or in response to a *price/tax* to emit CO_2
- intended to be used by *scientists*, CCS *stakeholders*, *policy makers*, and general *public*

Scenario

- *overbuilds infrastructure* (e.g., pipelines, capture) in early periods to achieves *long-term economies of scale*
- overall *CCS costs rise through time* as more expensive CO_2 sources are brought online, *transport costs fall* through increased utilization (Chart A)
- *SimCCS^{TIME}* balances CCS costs across *all time periods* while *minimizing costs* in any one time period (Chart B)

Middleton *et al.* (2012) A dynamic model for optimally phasing in CO_2 capture and storage infrastructure, *Environment Modelling & Software*

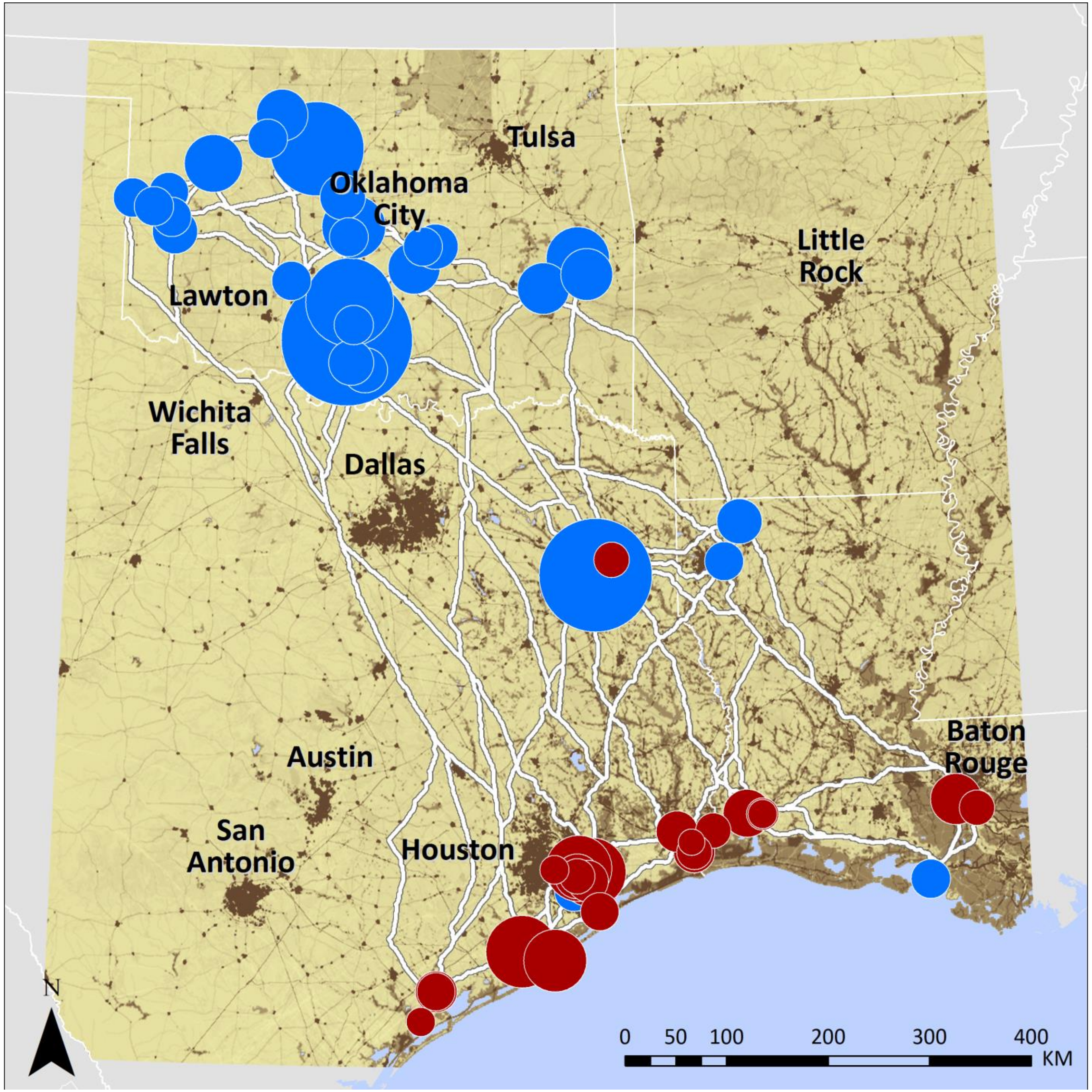
(4) Linear Model

Ethylene and CO_2-EOR

- Industrial source of CO_2.
- Market for CO_2 (i.e., CO_2-EOR).

Linearized pipelines

- Massively reduces the number of discrete variables (hard to solve for) and constraints.
- Reduces solution times between one to two orders of magnitude.



Middleton (2012) A new optimization approach to energy network modeling: anthropogenic CO_2 capture coupled with enhanced oil recovery, *International Journal of Energy Research*

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MODELS/APPLICATIONS

(5) *SimCCS*$^{2.0}$

Complete redesign

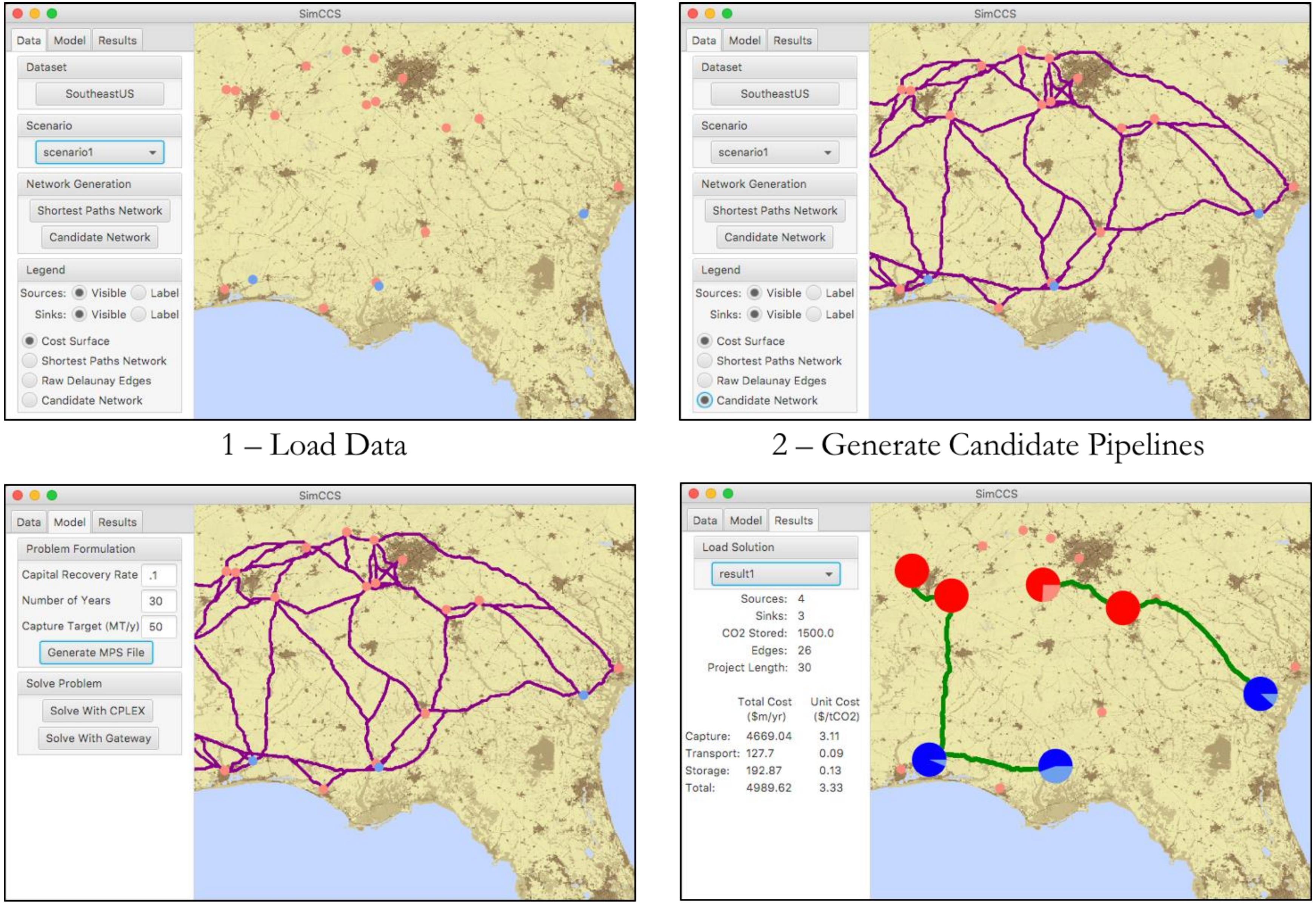
- Open source.
- Java based (multi-platform).
- HPC-enabled.
- Pug-and-play code.

Public domain

- “Business model” rethink.
- Enable collaborations.
- Multi-institutional efforts.
- https://github.com/SimCCS/SimCCS.

Cost surface

- Beta code integrated into *SimCCS* for the first time.



1 – Load Data

2 – Generate Candidate Pipelines

3 – Formulate Optimization Problem

4 – Display Solution

Middleton *et al.* (2018) An open-source tool for optimizing CO_2 capture, transport, and storage infrastructure, *Environmental Modelling & Software (in review)*

CarbonSAFEs (Los Alamos)

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Phase I (wrapped)

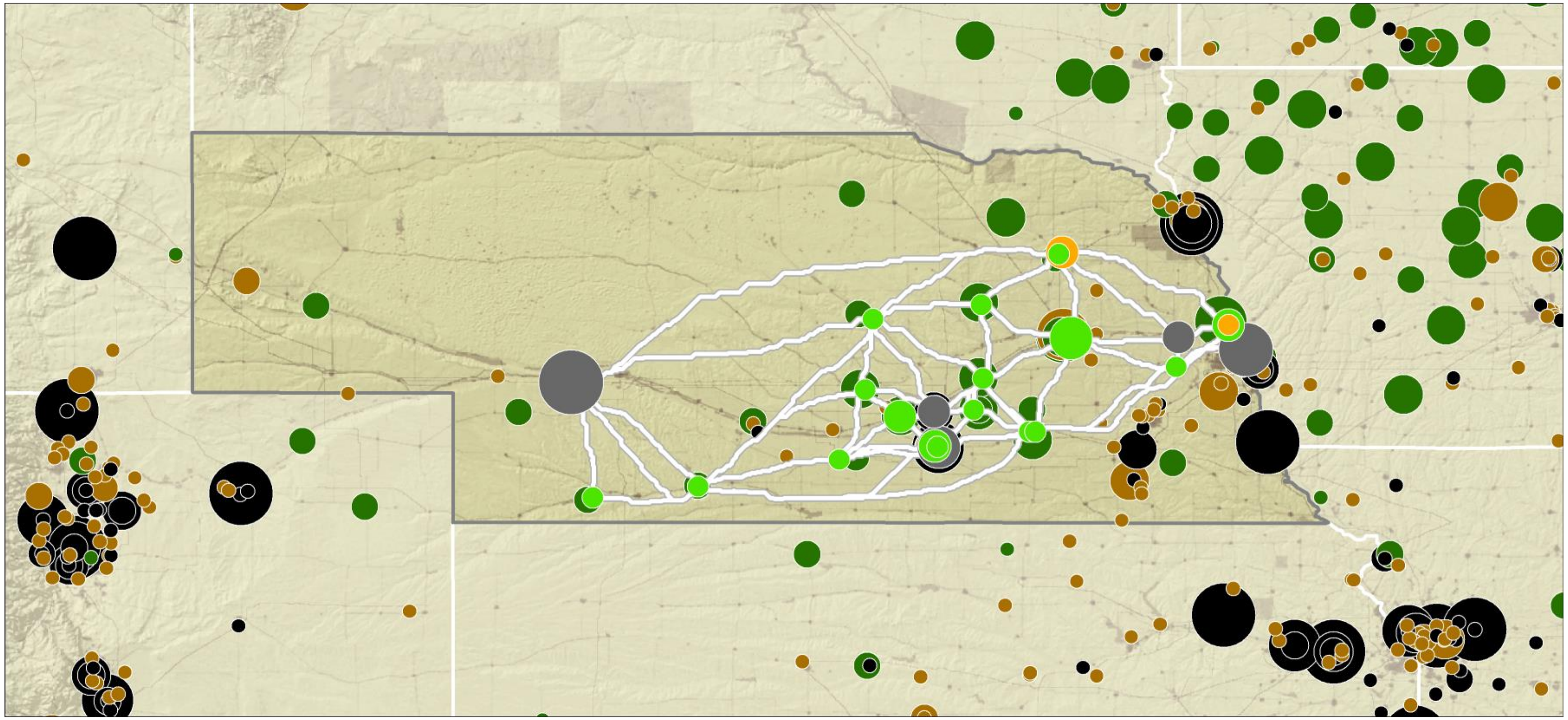
- Rocky Mountain (University of Utah).
- Nebraska (Battelle).
- Ohio (Battelle).
- Michigan (Battelle).

Phase II

- Nebraska+ (Battelle).
- US Southeast (SSEB).

Nebraska CCS Complex

- Integrated Mid-Continent Stacked Carbon Storage Hub.
- Prototype project to jumpstart commercial-scale CCUS?



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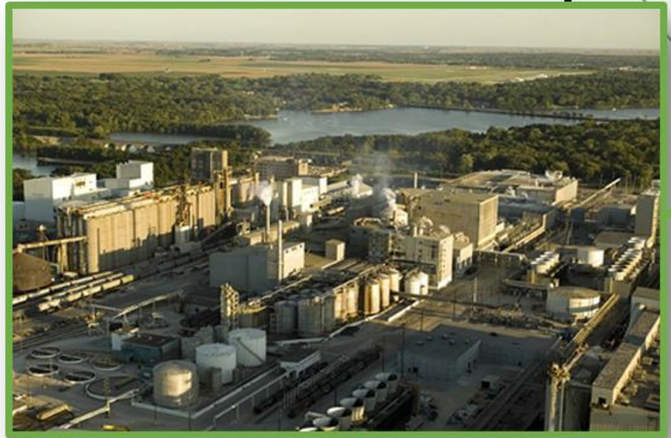
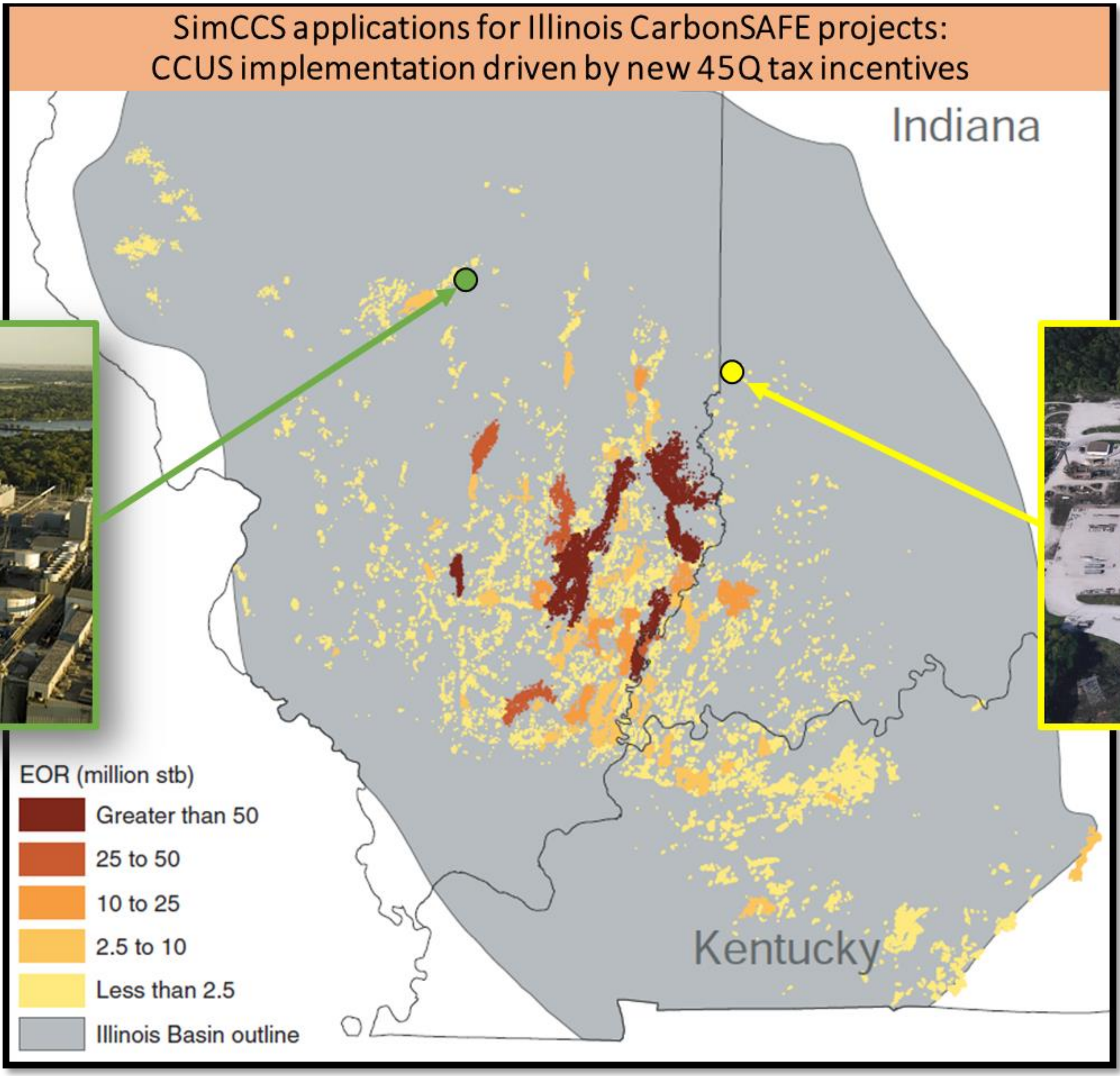
CarbonSAFEs (Indiana University)



IL ICCS Project
Ethanol from Corn
Currently 1 million tons of CO_2 capture annually
$208 Million
(USDOE-$141M, ADM-$67M)



Quasar Wabash Project
Ammonia from Coal Syngas
Expect ~ 2 million tons of CO_2 annually
$450 Million (all private)

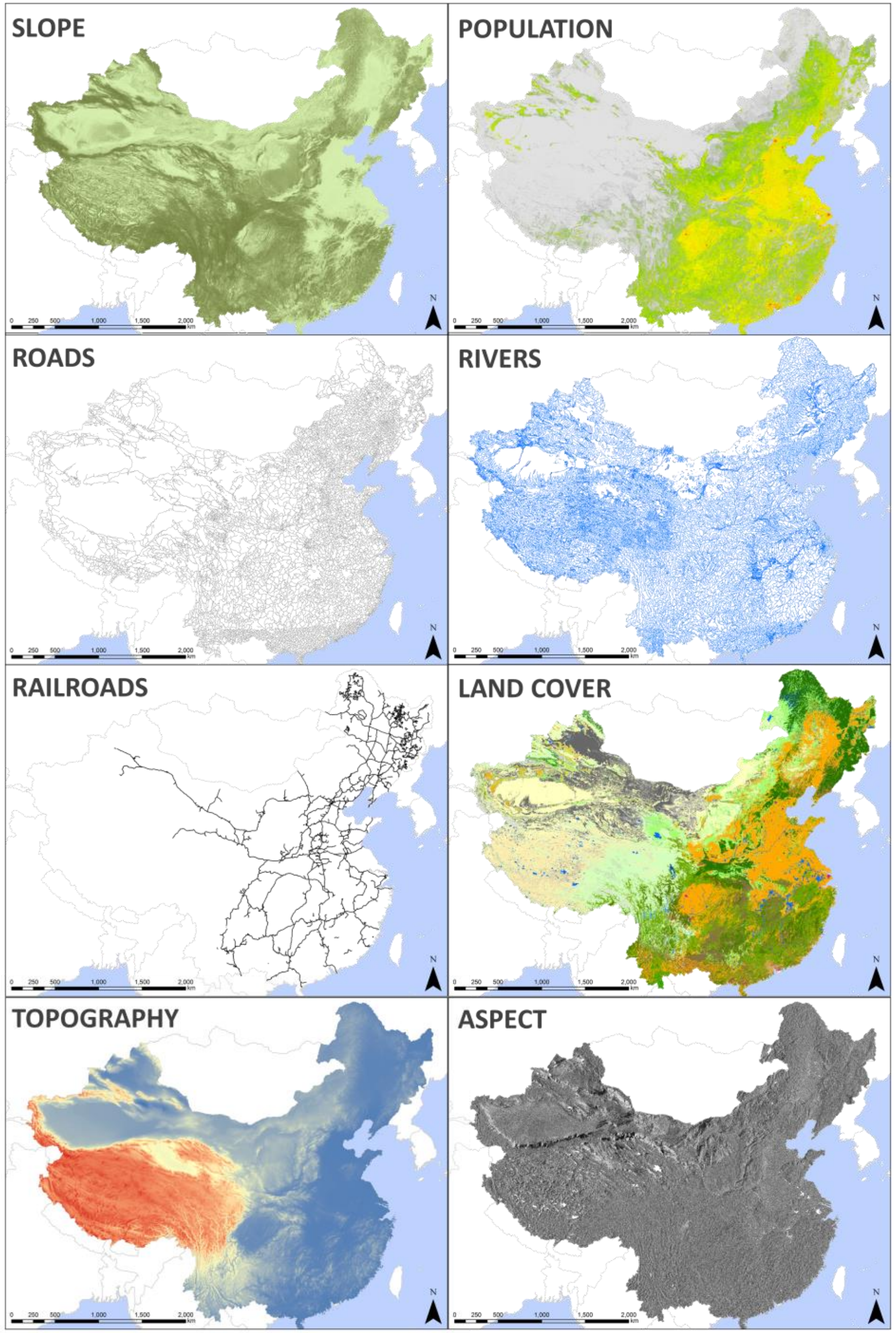
China

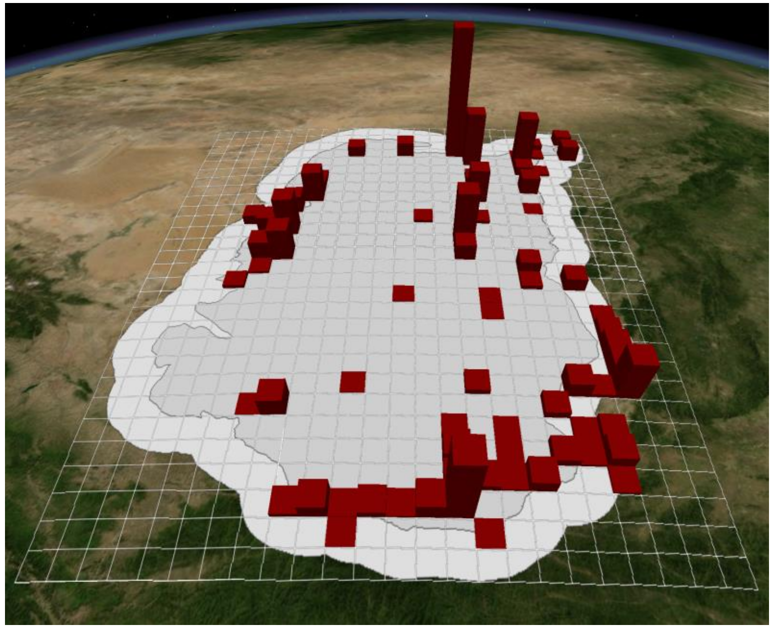
US-China CERC-ACTC

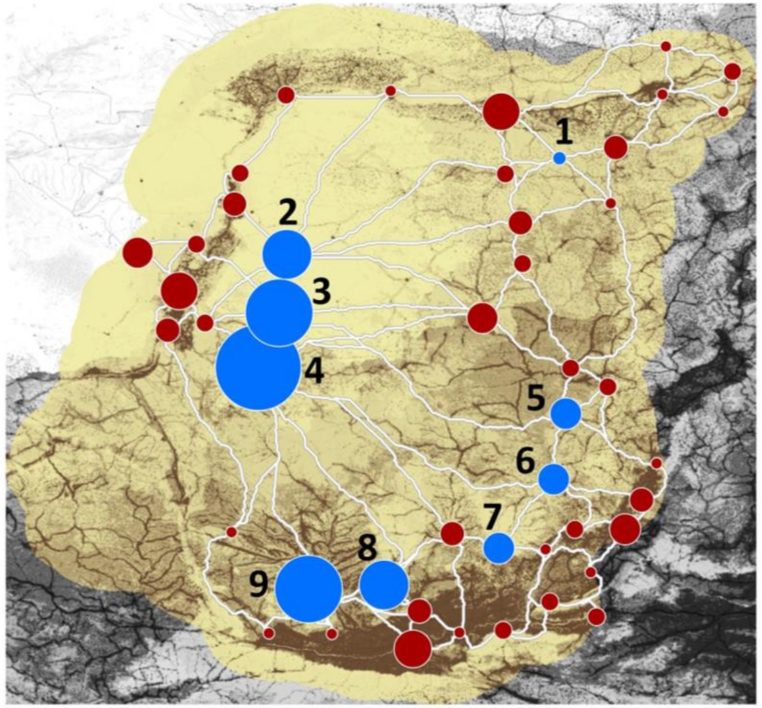
- Clean Energy Research Center (CERC) for Advanced Coal Technologies Consortium (ACTC).
- Collaboration with Chinese Academy of Sciences.

Logistics

- 290 sources emitting 350 $MtCO_2$/yr.
- Large saline storage opportunities, minimal utilization options.
- China-wide cost surface.







Stauffer *et al.* (2014) System integration linking CO_2 sources, sinks, and infrastructure for the Ordos Basin, China, *Energy Procedia*

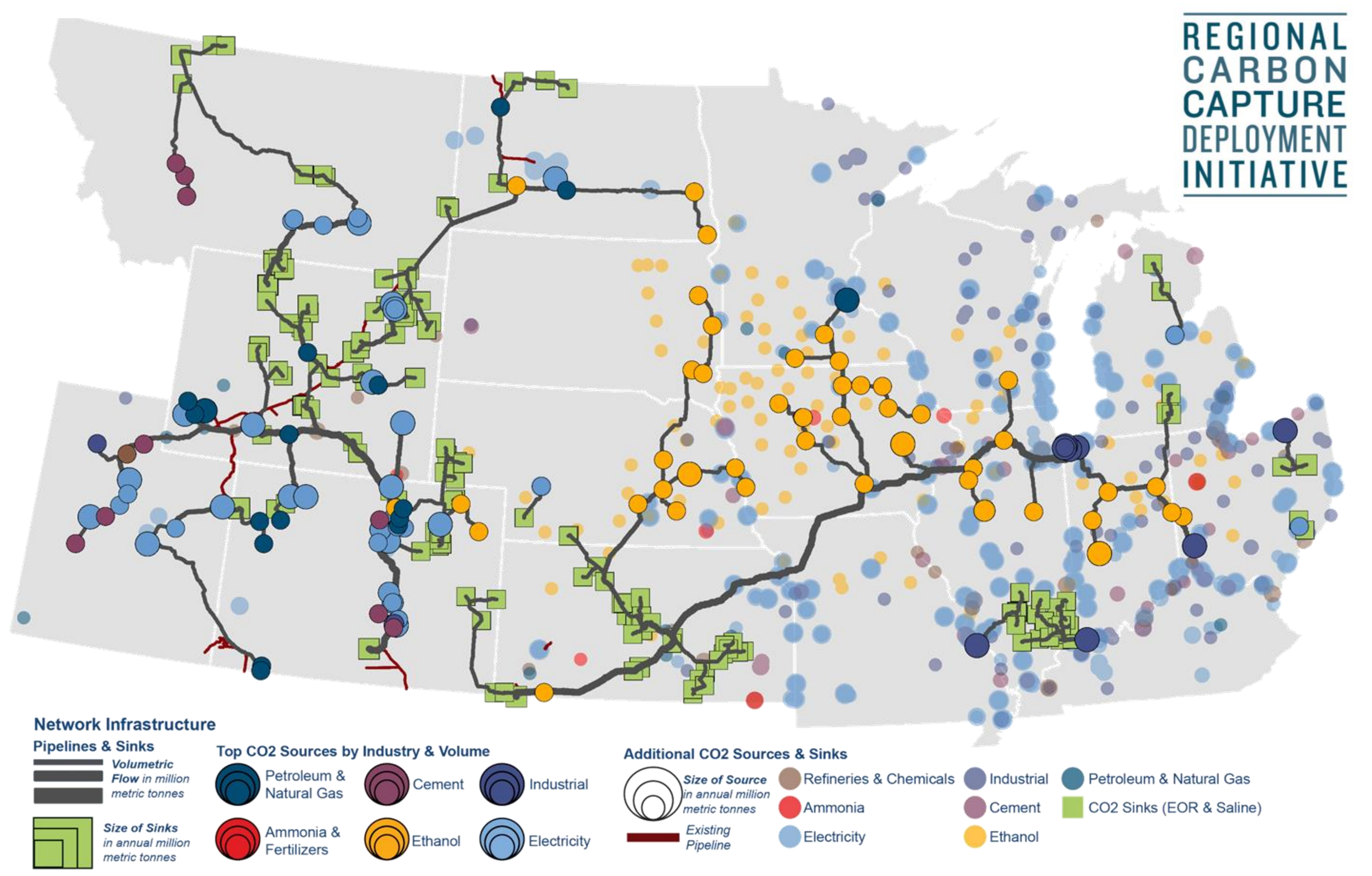
State Carbon Capture Work Group

Carbon Capture Coalition

“,,,realize carbon capture’s full potential as a national energy, economic, and environmental strategy.”

Regional Carbon Capture Deployment Initiative

- MT and WY governors.
- Capitalize on 45Q tax credit.
- Nationwide mapping, identify low-cost CO_2 capture projects.
- State-led efforts.



http://www.betterenergy.org/blog/press-release-14-state-work-group-releases-federal-state-recommendations-carbon-capture/

CONTACT: Brad Crabtree; bcrabtree@gpisd.net.

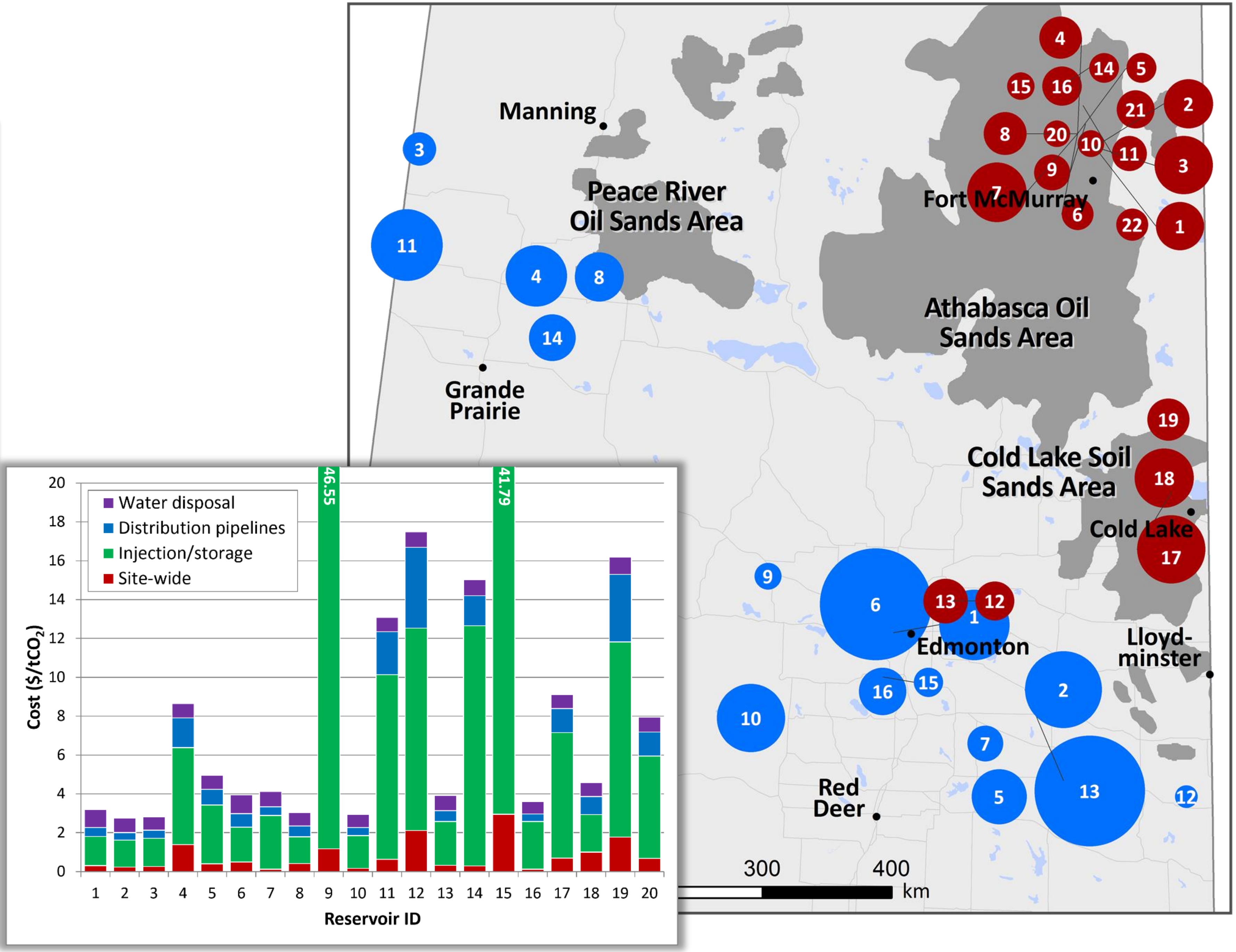
Uncertainty

Geologic uncertainty

- SCO_2T (NRAP-IAM): → injection rate & storage.
- Formation thickness, permeability, and porosity.
- *SimCCS*: uncertainty impact on injection/storage costs.

Impact

- **PERMEABILITY:** injectivity → number of wells → cost.
- **POROSITY:** pore space → fix site costs.
- Correlated permeability and porosity in similar formations.
- **TIPPING POINT:** ~0.25 $MtCO_2$/yr (due to number of required wells).



Middleton and Yaw (2018) The Cost of Getting CCS Wrong, *International Journal of Greenhouse Gas Control*

Current Projects

Uncertainty

Geologic uncertainty

- SCO_2T (NRAP-IAM): → injection rate & storage.
- Formation thickness, permeability, and porosity.
- *SimCCS*: uncertainty impact on injection/storage costs.

Impact

- **Permeability:** injectivity → number of wells → cost.
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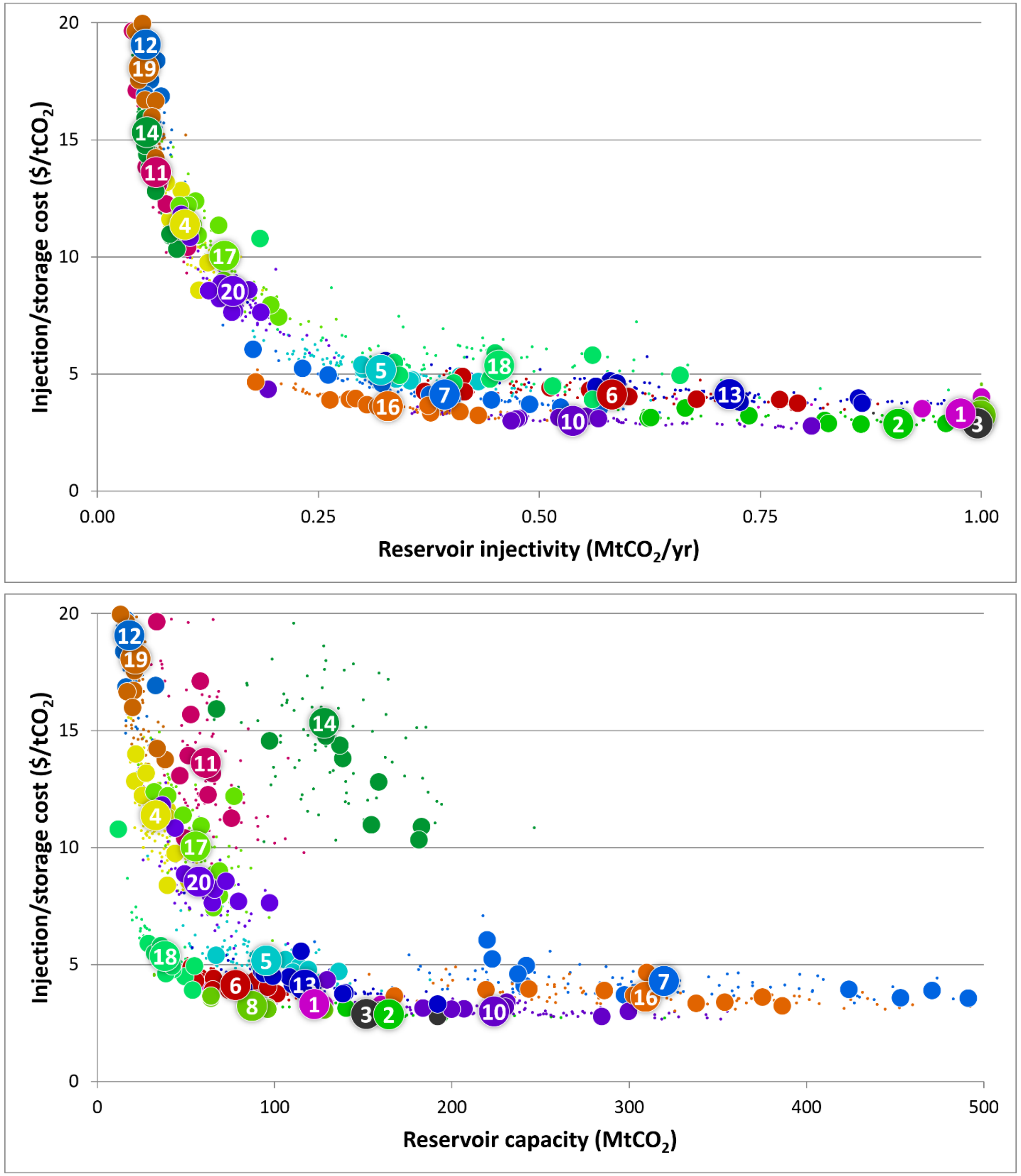

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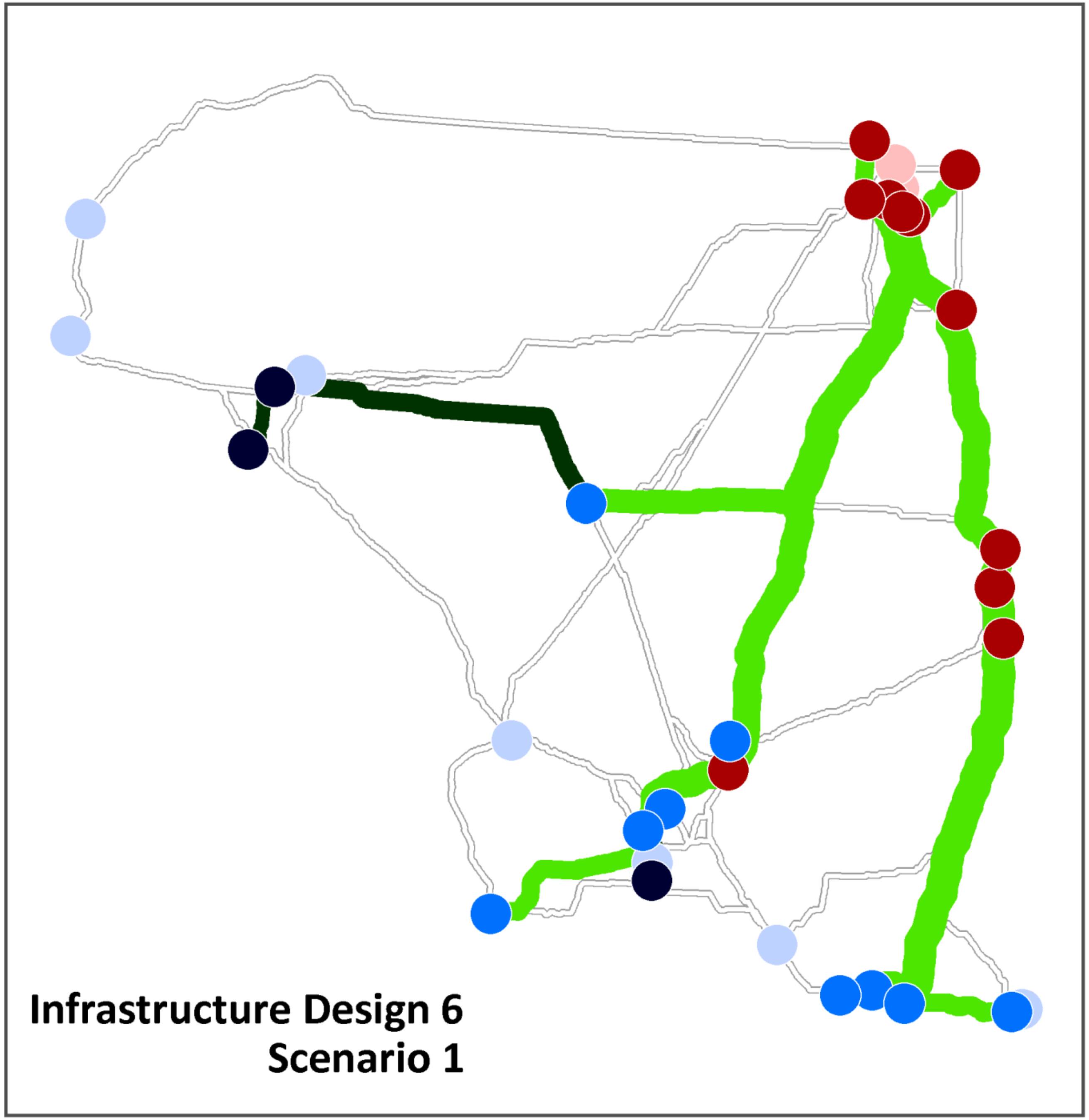
Uncertainty

Results

- New infrastructure required to make solutions feasible (i.e., “stranded CO_2”).
- Dramatic differences in CCS infrastructure and costs.
- Duplicated infrastructure.

Stranded CO_2

- Penalty for not emitting “excess” CO_2.
- 1–2 years CO_2 tax transforms best solution into worst case.
- Design resilient infrastructure?



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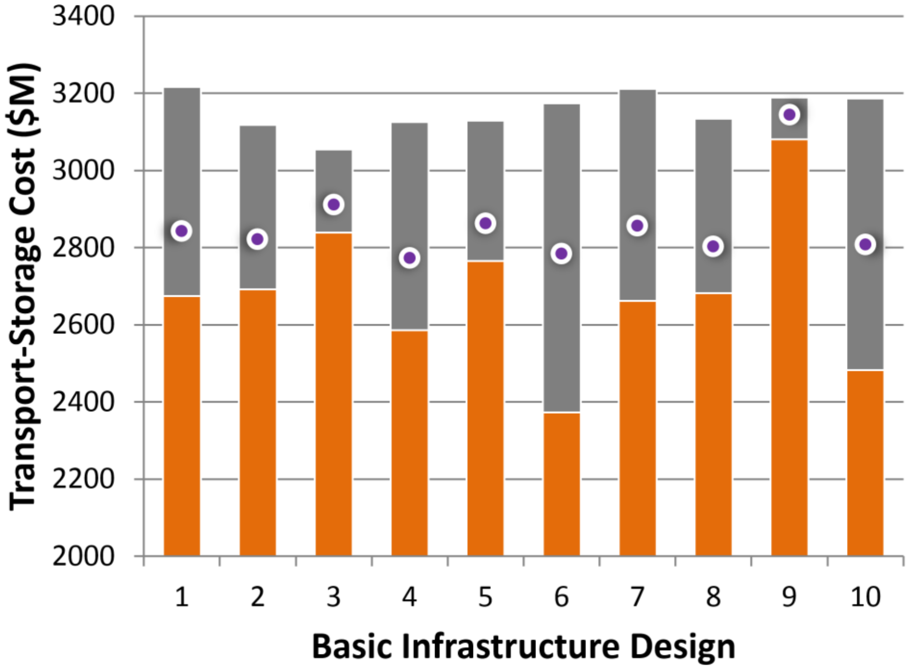

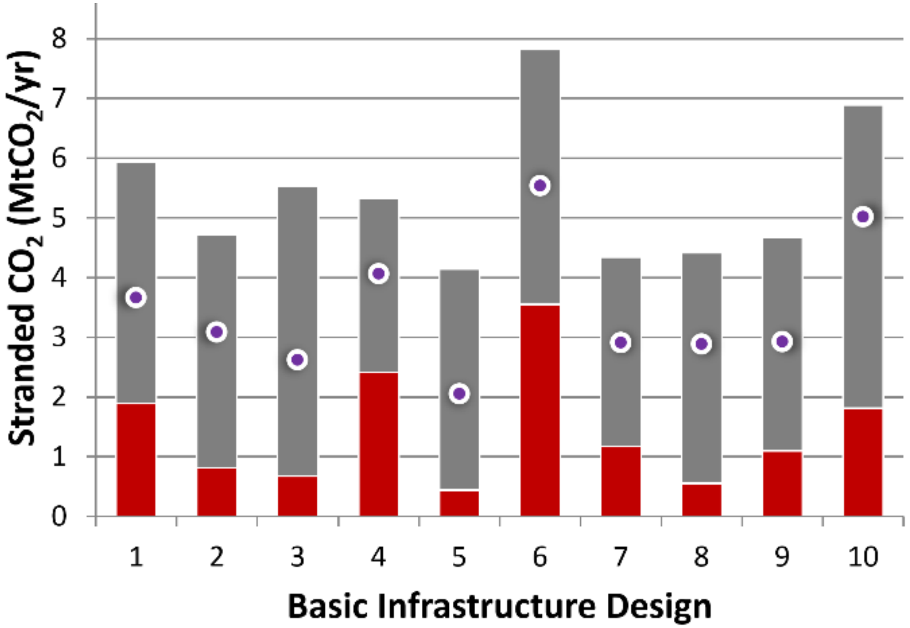

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New Approach: Endogenously Handling Uncertainty

$$\overbrace{\sum_{i\in S} F_i^s s_i^b + \sum_{k\in K}\sum_{c\in C}\beta_{kc} y_{kc}^b + \sum_{j\in R}\sum_{u\in U} F_j^r r_{ju}^b}^{\text{base design cost}} + \overbrace{\frac{1}{|U|}\left(\sum_{u\in U}\sum_{i\in S}(F_i^s s_{iu} + V_i^s a_{iu}) + \sum_{u\in U}\sum_{k\in K}\sum_{c\in C}\alpha_{kc} p_{kcu} + \sum_{u\in U}\sum_{k\in K}\sum_{c\in C}\beta_{kc} y_{kcu} + \sum_{u\in U}\sum_{j\in R}(F_j^r r_{ju} + V_j^r b_{ju})\right)}^{\text{average uncertain delta costs}}$$

Source/Sink opening & pipeline construction costs

Network utilization + construction for uncertain parameters.

Model Update: Design network that intrinsically accounts for uncertain parameters.

$Q_{kc}^{\min}(y_{kcu} + y_{kc}^b) \le p_{kcu} \le Q_{kc}^{\max}(y_{kcu} + y_{kc}^b), \forall k\in K, \forall c\in C, \forall u\in U$	Pipeline capacity compatible with flow volume for delta designs
$Q_{kc}^{\min} y_{kc}^b \le p_{kc}^b \le Q_{kc}^{\max} y_{kc}^b, \forall k\in K, \forall c\in C$	Pipeline capacity compatible with flow volume for base design
$\sum_{k\in K: src(k)=i}\sum_{c\in C} p_{kcu} - \sum_{k\in K: dst(k)=i}\sum_{c\in C} p_{kcu} = \begin{cases} a_{iu} & i\in S \\ -b_{iu} & i\in R \\ 0 & \text{otherwise}\end{cases}, \forall i\in I, \forall u\in U$	Conservation of flow for delta designs
$\sum_{k\in K: src(k)=i}\sum_{c\in C} p_{kc}^b - \sum_{k\in K: dst(k)=i}\sum_{c\in C} p_{kc}^b = \begin{cases} a_i^b & i\in S \\ -b_i^b & i\in R \\ 0 & \text{otherwise}\end{cases}, \forall i\in I$	Conservation of flow for base design
$a_{iu} \le Q_i^s(s_{iu} + s_i^b), \forall i\in S, \forall u\in U$	Source capture capped by maximum production for delta designs
$a_i^b \le Q_i^s s_i^b, \forall i\in S$	Source capture capped by maximum production for base design
$b_{ju} \le Q_{ju}^r\left(r_{ju} + \sum_{w\in U} r_{jw}^b\right), \forall j\in R, \forall u\in U$	Reservoir storage capped by maximum capacity for delta designs
$b_j^b \le \sum_{u\in U} Q_{ju}^r r_{ju}^b, \forall j\in R$	Reservoir storage capped by maximum capacity of base parameters
$r_{ju}^b \le v_u, \forall j\in R, \forall u\in U$	Set base design uncertainty parameter selection variables
$\sum_{u\in U} v_u \le 1$	Single uncertainty parameter selected for base network
$\sum_{i\in S} a_{iu} \ge CO_2Cap, \forall u\in U$	Total captured meets target for delta designs
$\sum_{i\in S} a_i^b \ge CO_2Cap$	Total captured meets target for base network
$s_{iu} + s_i^b \le 1, \forall i\in S, \forall u\in U$	Source opened at most once
$y_{kcu} + y_{kc}^b \le 1, \forall k\in K, \forall c\in C, \forall u\in U$	Edge opened at most once
$r_{ju} + \sum_{w\in U} r_{jw}^b \le 1, \forall j\in R, \forall u\in U$	Reservoir opened at most once

Capability: Generates robust solution given uncertain parameters.

Middleton and Yaw (2018) The Cost of Getting CCS Wrong, *International Journal of Greenhouse Gas Control*

New Approach: Endogenously Handling Uncertainty

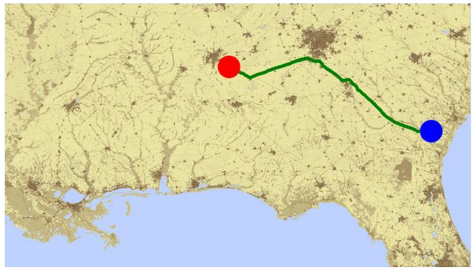
New Model Performance

- Able to leverage intelligent overbuilding not explored by previous methods.
- Proof-of-concept scenario yields 16% cost savings for new model over previous methods.

Existing model with previous uncertainty methods.

Optimal for parameter set 1

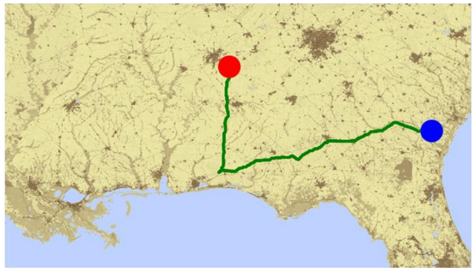
Extended to parameter set 2



Optimal for parameter set 2

Extended to parameter set 1

New model with intrinsic uncertainty handling.



Optimal for parameter set 2

Extended to parameter set 1

Uncertainty: Endogneously Handling Uncertainty

$$\overbrace{\sum_{i\in S} F_i^s s_i^b + \sum_{k\in K}\sum_{c\in C} \beta_{kc} y_{kc}^b + \sum_{j\in R}\sum_{u\in U} F_j^r r_{ju}^b}^{\textit{base design cost}} + \overbrace{\frac{1}{|U|}\left(\sum_{u\in U}\sum_{i\in S}\left(F_i^s s_{iu} + V_i^s a_{iu}\right) + \sum_{u\in U}\sum_{k\in K}\sum_{c\in C} \alpha_{kc} p_{kcu} + \sum_{u\in U}\sum_{k\in K}\sum_{c\in C} \beta_{kc} y_{kcu} + \sum_{u\in U}\sum_{j\in R}\left(F_j^r r_{ju} + V_j^r b_{ju}\right)\right)}^{\textit{average uncertain delta costs}}$$

Source/Sink opening & pipeline construction costs

Network utilization + construction for uncertain parameters.

Model Update: Design network that intrinsically accounts for uncertain parameters.

Capability: Generates robust solution given uncertain parameters.

$Q_{kc}^{\min}(y_{kcu} + y_{kc}^b) \le p_{kcu} \le Q_{kc}^{\max}(y_{kcu} + y_{kc}^b), \forall k \in K, \forall c \in C, \forall u \in U$	Pipeline capacity compatible with flow volume for delta designs
$Q_{kc}^{\min} y_{kc}^b \le p_{kc}^b \le Q_{kc}^{\max} y_{kc}^b, \forall k \in K, \forall c \in C$	Pipeline capacity compatible with flow volume for base design
$\sum_{\substack{k\in K:\\ src(k)=i}}\sum_{c\in C} p_{kcu} - \sum_{\substack{k\in K:\\ dst(k)=i}}\sum_{c\in C} p_{kcu} = \begin{cases} a_{iu} & i \in S \\ -b_{iu} & i \in R \\ 0 & \text{otherwise} \end{cases}, \forall i \in I, \forall u \in U$	Conservation of flow for delta designs
$\sum_{\substack{k\in K:\\ src(k)=i}}\sum_{c\in C} p_{kc}^b - \sum_{\substack{k\in K:\\ dst(k)=i}}\sum_{c\in C} p_{kc}^b = \begin{cases} a_i^b & i \in S \\ -b_i^b & i \in R \\ 0 & \text{otherwise} \end{cases}, \forall i \in I$	Conservation of flow for base design
$a_{iu} \le Q_i^s(s_{iu} + s_i^b), \forall i \in S, \forall u \in U$	Source capture capped by maximum production for delta designs
$a_i^b \le Q_i^s s_i^b, \forall i \in S$	Source capture capped by maximum production for base design
$b_{ju} \le Q_{ju}^r\left(r_{ju} + \sum_{w\in U} r_{jw}^b\right), \forall j \in R, \forall u \in U$	Reservoir storage capped by maximum capacity for delta designs
$b_j^b \le \sum_{u\in U} Q_{ju}^r r_{ju}^b, \forall j \in R$	Reservoir storage capped by maximum capacity of base parameters
$r_{ju}^b \le v_u, \forall j \in R, \forall u \in U$	Set base design uncertainty parameter selection variables
$\sum_{u\in U} v_u \le 1$	Single uncertainty parameter selected for base network
$\sum_{i\in S} a_{iu} \ge CO_2\text{Cap}, \forall u \in U$	Total captured meets target for delta designs
$\sum_{i\in S} a_i^b \ge CO_2\text{Cap}$	Total captured meets target for base network
$s_{iu} + s_i^b \le 1, \forall i \in S, \forall u \in U$	Source opened at most once
$y_{kcu} + y_{kc}^b \le 1, \forall k \in K, \forall c \in C, \forall u \in U$	Edge opened at most once
$r_{ju} + \sum_{w\in U} r_{jw}^b \le 1, \forall j \in R, \forall u \in U$	Reservoir opened at most once

Middleton and Yaw (2018) The Cost of Getting CCS Wrong, *International Journal of Greenhouse Gas Control*

SimCCS: Development and Applications

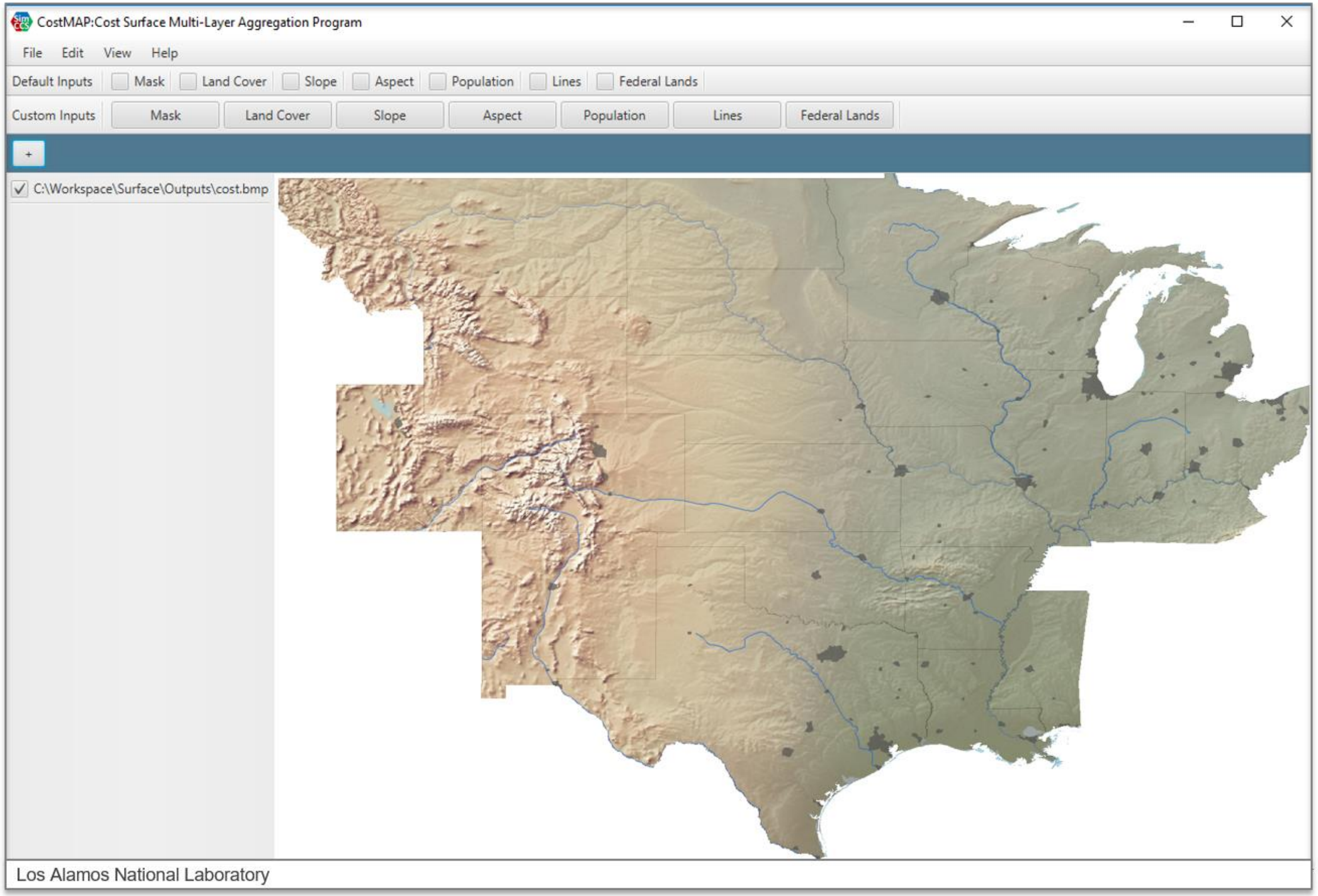
New project

- DOE Fossil Energy.
- Started September 2018.

Tasks:

1. New cost surface science and tools (CostMAP).
2. Develop meta-heuristic to solve complex problems and large domains.
3. Preparation for R&D100.

CostMAP: Cost Surface Multi-Aggregation Program

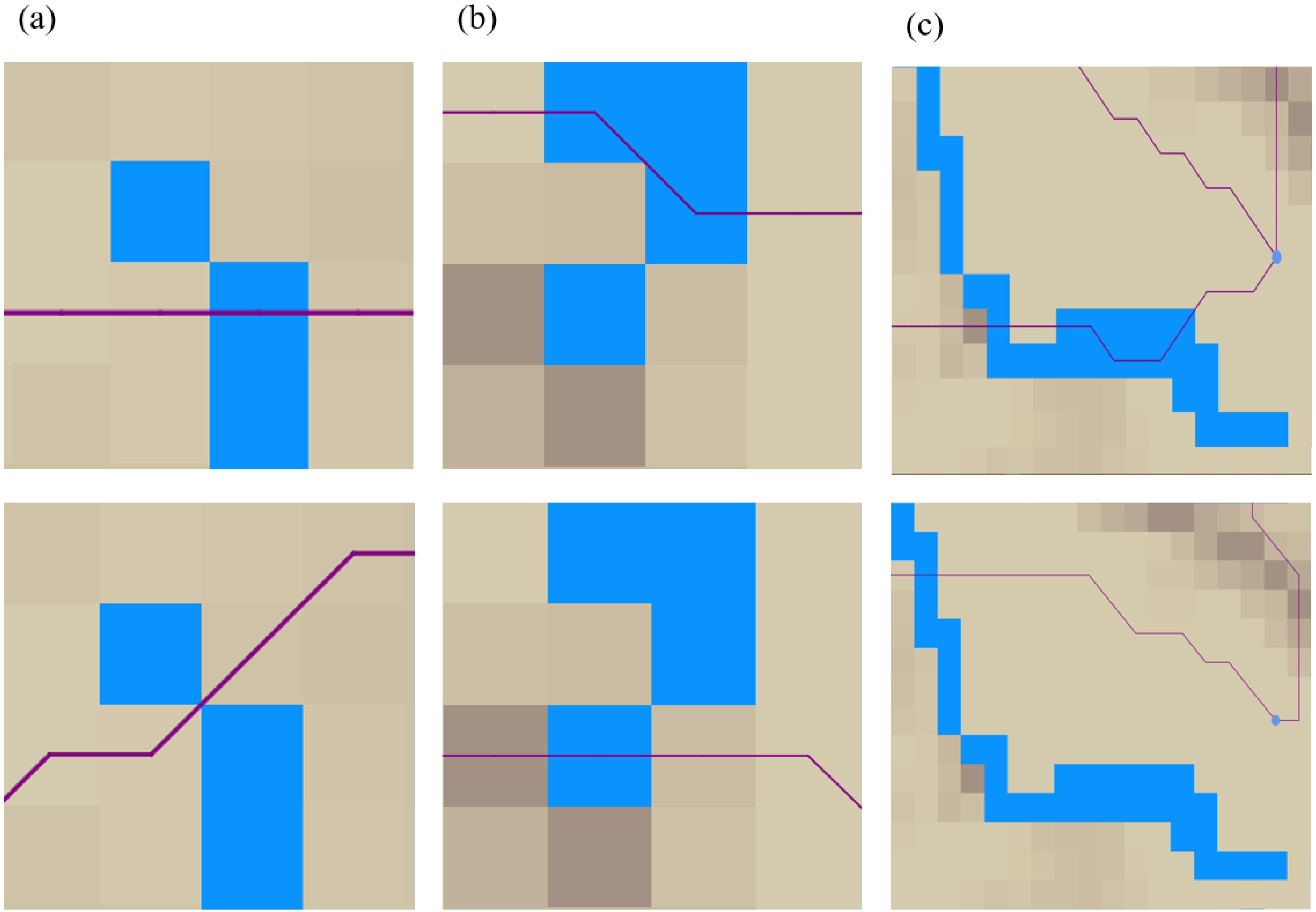


CostMAP: Cost Surface Multi-layer Aggregation Program

Improved Accuracy

Identifies barriers more accurately.

- **Top** shows the results from a traditional kernel.
- **Bottom** shows the results from the search kernel in CostMAP.

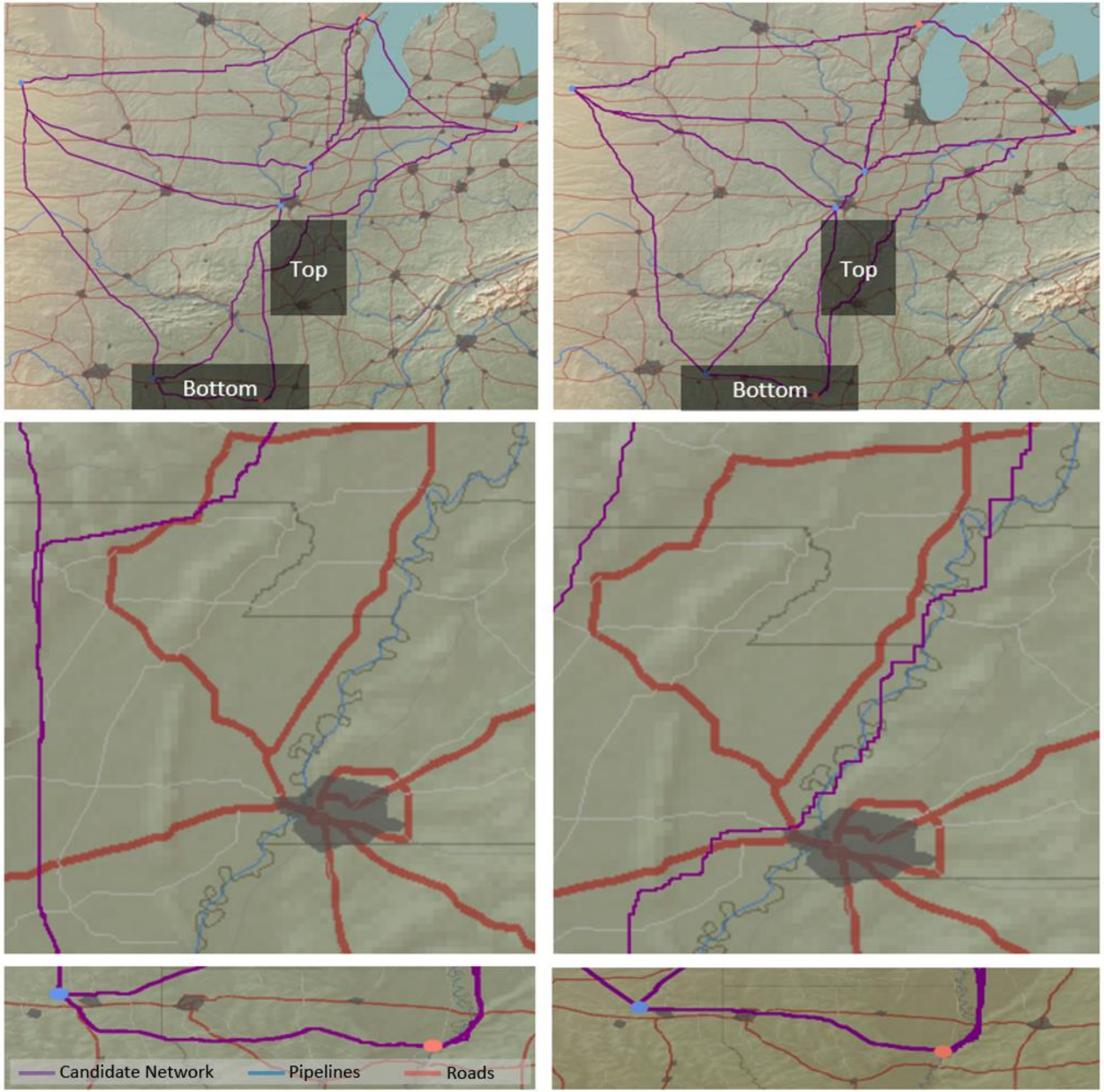


CURRENT PROJECTS
CostMAP

Improved Accuracy

Identifies corridors more accurately.

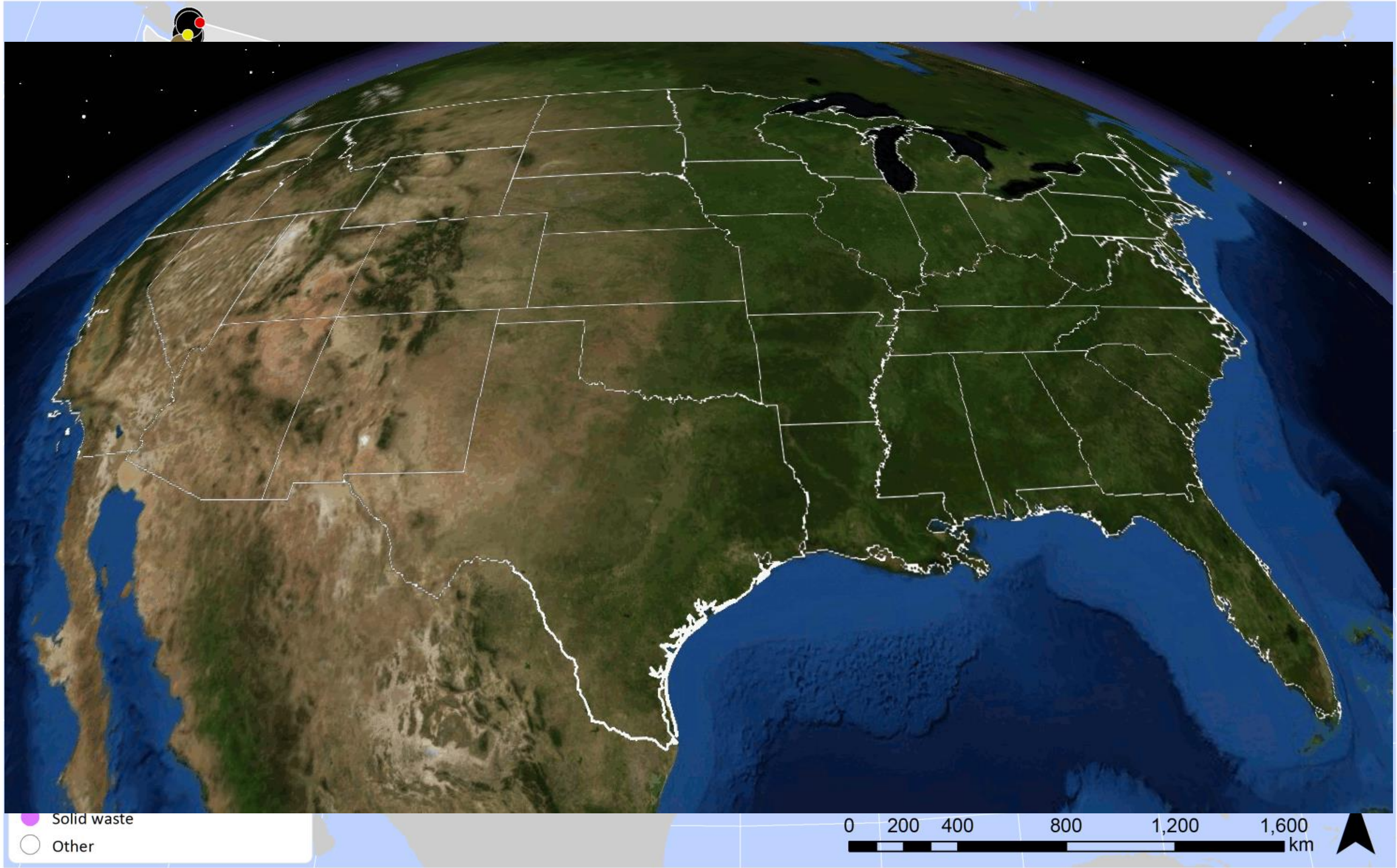
- **LEFT** shows the results from a traditional kernel.
- **RIGHT** shows the results from the search kernel in CostMAP.



SCO_2NE

Power and industrial sources of CO_2

- Sources of CO_2 that are not electricity (SCO_2NE)!
- Industrial and power CO_2 emissions → EPA GHG and other sources.

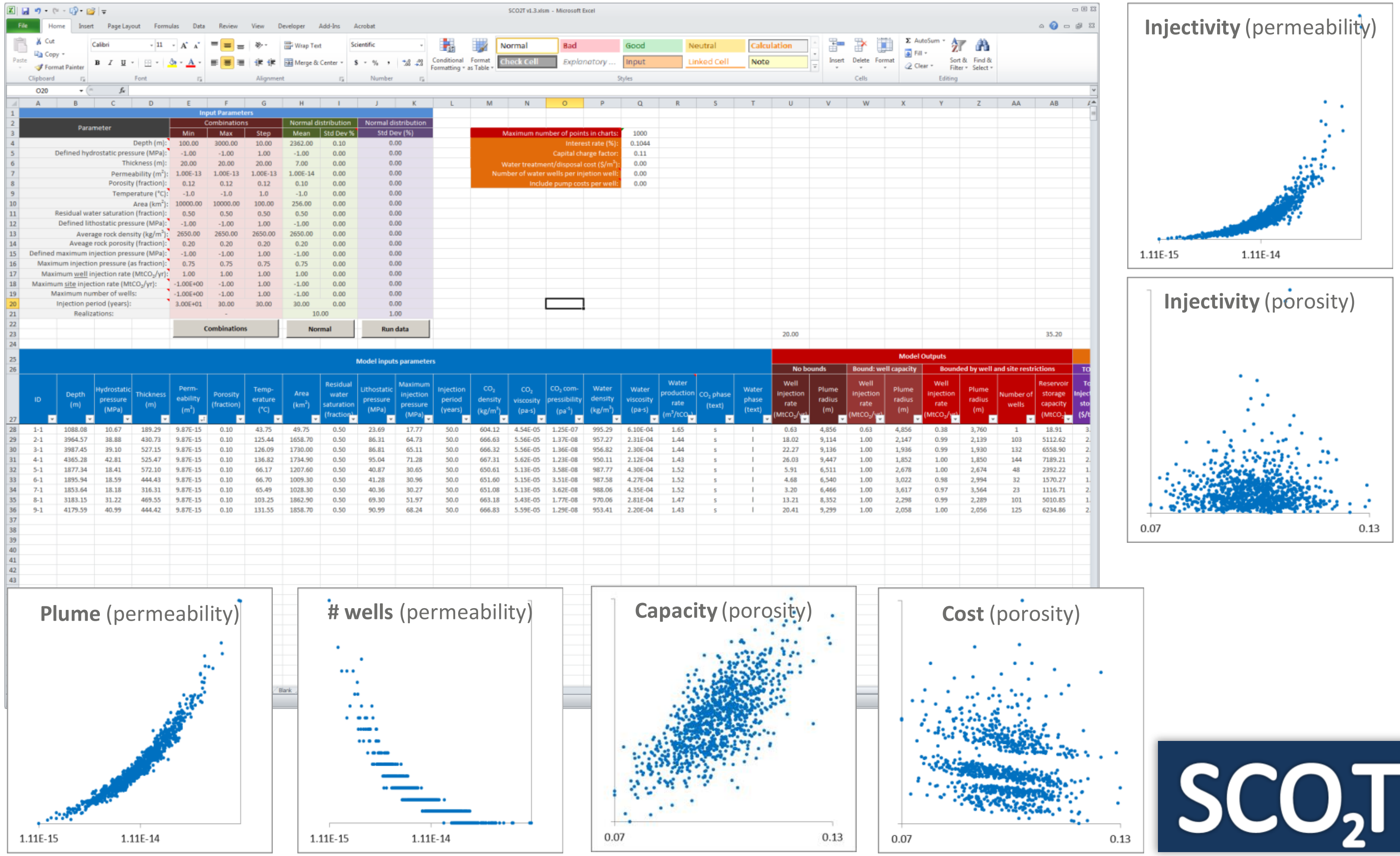


Middleton *et al.* (2017) Industrial CO_2 and carbon capture: near-term benefit, long-term necessity, *Energy Procedia*

Great SCO_2T!

Sequestration of CO_2 Tool (SCO_2T)

- Excel-based tool for Windows and Macs (no installation!).
- Reduced order models trained by multiphase physics (i.e., FEHM).
- Integrated with SimCCS' storage economic model (i.e., SCO_2T exports *SimCCS*-ready storage input data).



Middleton (2014) Secure and sustainable energy infrastructure: The case of CO_2 capture, utilization, and storage, LA-UR-14-21812

LA-UR-18-29408

ALIGNED WORK
SimCCS Gateway

Science Gateway

- Indiana University thrust.
- Portal to *SimCCS* desktop or online *SimCCS*.
- High-performance computing (currently IU’s Big Red, ultimately could based).
- Dependent on *SimCCS* base developments.

SimCCS Gateway

SimCCS is a decision support tool for integrated assessment of carbon capture, utilization and storage technology developed by members of the U.S.-China Clean Energy Research Center, Advanced Coal Technology Consortium. SimCCS Gateway is a science gateway built from the collaboration between the Indiana Geological & Water Survey and the Science Gateways Group at Indiana University.

SimCCS supports decision making on CO_2 mitigation technology deployment by integrating applications in operations research, geographical information systems, CO_2 capture modelling, pipeline engineering design, and reservoir engineering and geology. At its core, SimCCS is driven by a mixed-integer linear programming optimization engine for obtaining solutions that drive model decisions.

SimCCS produces optimal solutions for integrated CCUS infrastructure deployment in three different modes:
(1) $SimCCS^{CAP}$: the model is given an exogenously-defined amount of CO_2 to capture across one or more CO_2-emitting sources. Consequently, SimCCS designs the least-cost set of infrastructure to manage the desired CO_2 target. This is considered to be the version of SimCCS to operate within an emissions cap, or cap-and-trade environment. Alternatively, the user can define a fixed budget and let the ... that can be managed within that

... in response to a price (or tax) on ... ucture and managing CO_2 flows at ... nosphere. ... aspect to infrastructure ... discrete time steps. The model can ... RICE mode.

SimCCS has been developed as a desktop-level, science-based research tool requiring intimate knowledge of the framework to effectively execute the program, as well as the application of external, proprietary software including ESRI’s ArcGIS and IBM’s CPLEX. Here we further develop SimCCS to run on high-performance computing platforms such that robust optimal solutions can be obtained in the face of significant uncertainty. Toward this end, we will develop new algorithms and reduced-order solution methods that will allow thousands of SimCCS solutions to be analyzed to identify critical techno-economic thresholds in CCUS infrastructure deployment.

POWERED BY APACHE AIRAVATA

SimCCS Gateway is powered by Apache Airavata. Apache Airavata is a software framework which is dominantly used to build Web-based science gateways and assist to compose, manage, execute and monitor large scale applications and workflows on distributed computing resources such as local clusters, supercomputers, national grids, academic and commercial clouds. Airavata mainly supports long running applications and workflows on distributed computational resources.

Contact Us

You can contact Gateway Admin by sending a mail to Contact E-mail

WEBSITE: https://simccs.org/

LA-UR-18-29408

Take Home Message

Questions?

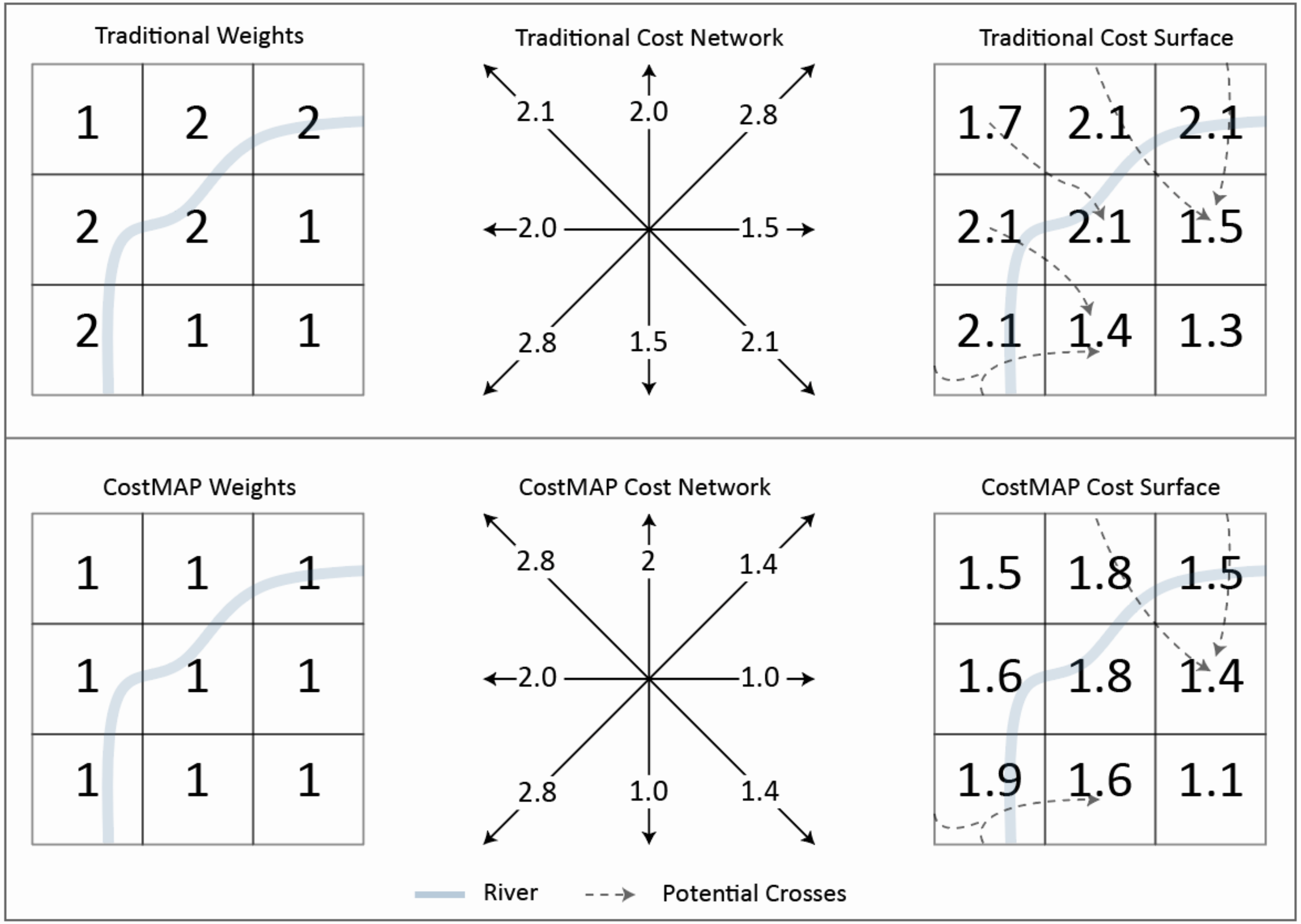
CostMAP: Comparison of cost calculation

Top

- Cost surface and cost Network calculation in most GIS programs.

Bottom

- Cost surface and Cost network calculation in CostMAP.

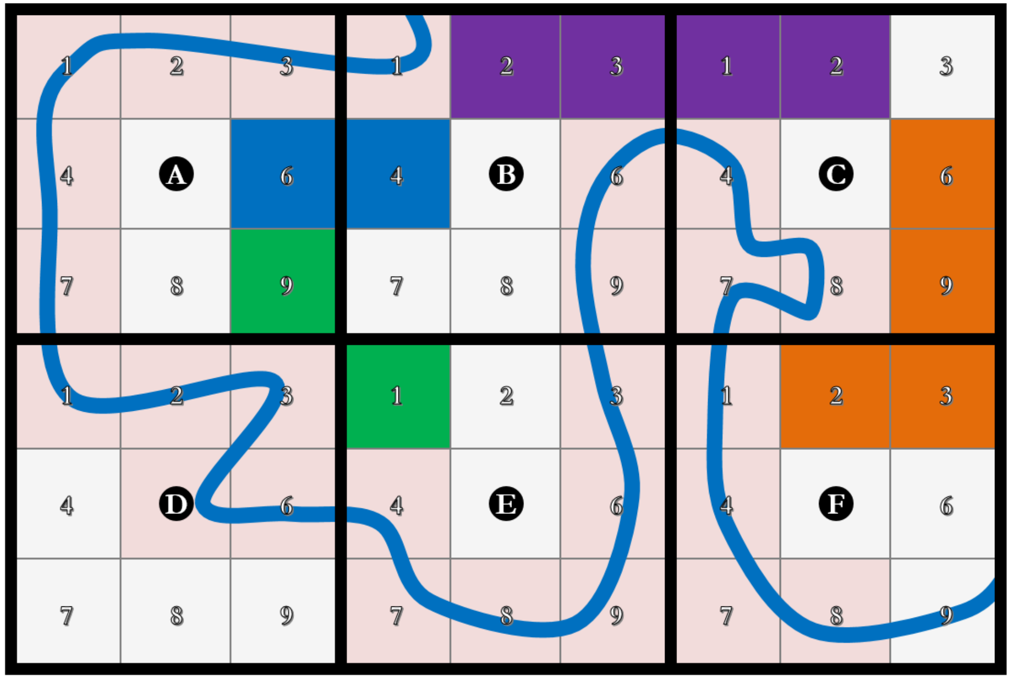


LA-UR-18-29408

CostMAP: Search Kernel Rules

Los Alamos NATIONAL LABORATORY EST. 1943

Barriers



Corridors